



## Full wwPDB EM Validation Report ⓘ

Oct 19, 2026 – 04:52 pm BST

PDB ID : 9T0I / pdb\_00009t0i  
EMDB ID : EMD-55401  
Title : Spraguea lophii ribosome dimer, conformation 1.  
Authors : McLaren, M.; Isupov, M.N.; Daum, B.; Conners, R.  
Deposited on : 2025-10-17  
Resolution : 9.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

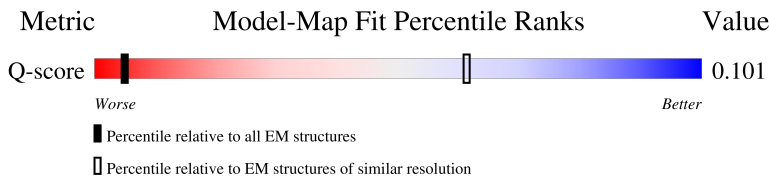
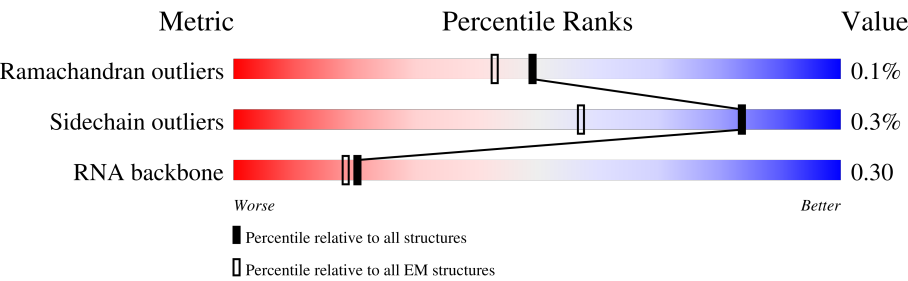
EMDB validation analysis : 0.0.1.dev133  
MolProbity : 4-5-2 with Phenix2.2  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.51

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 157 ( 9.30 - 10.30 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | K50   | 2618   |                  |
| 1   | L50   | 2618   |                  |
| 2   | R60   | 1368   |                  |
| 2   | S60   | 1368   |                  |

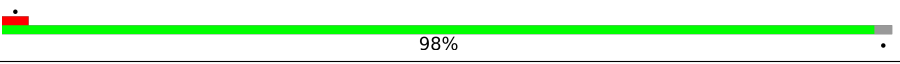
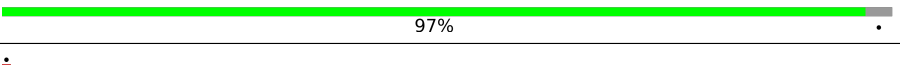
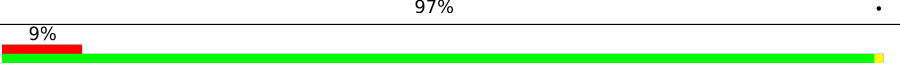
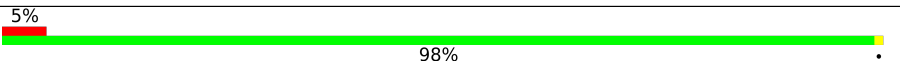
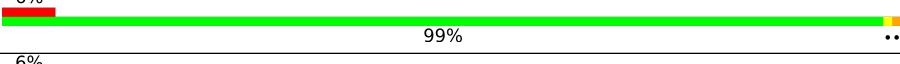
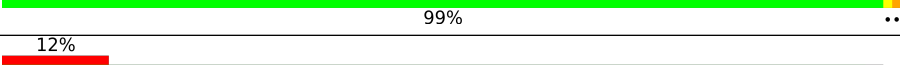
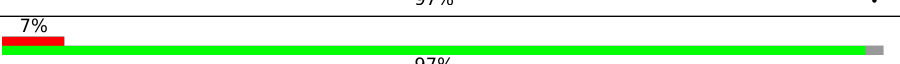
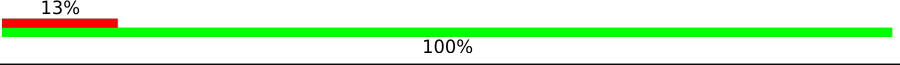
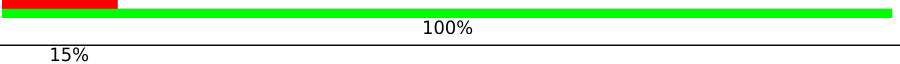
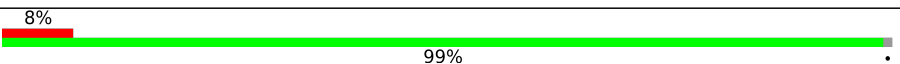
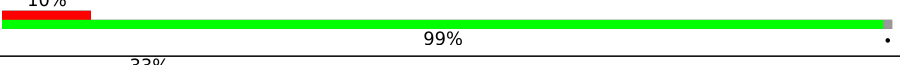
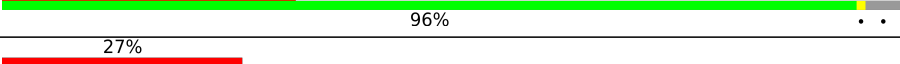
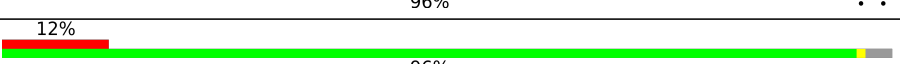
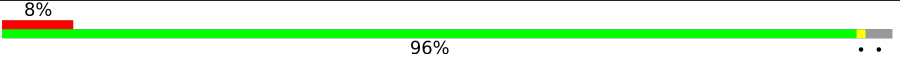
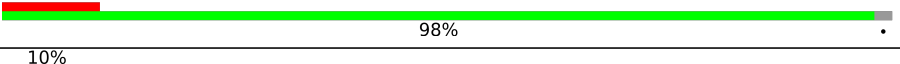
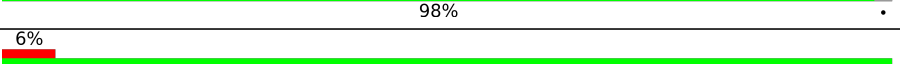
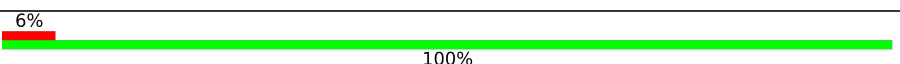
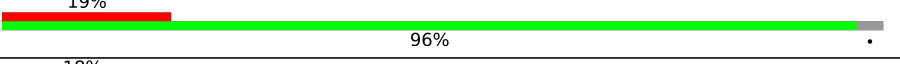
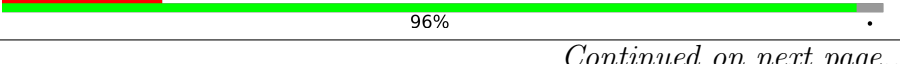
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | D     | 164    |                  |
| 3   | E     | 164    |                  |
| 4   | KGG   | 106    |                  |
| 4   | LGG   | 106    |                  |
| 5   | RB0   | 230    |                  |
| 5   | SB0   | 230    |                  |
| 6   | RC0   | 248    |                  |
| 6   | SC0   | 248    |                  |
| 7   | K70   | 119    |                  |
| 7   | L70   | 119    |                  |
| 8   | A     | 847    |                  |
| 8   | B     | 847    |                  |
| 9   | K     | 210    |                  |
| 9   | L     | 210    |                  |
| 10  | M     | 269    |                  |
| 10  | N     | 269    |                  |
| 11  | KMM   | 127    |                  |
| 11  | LMM   | 127    |                  |
| 12  | RBB   | 82     |                  |
| 12  | SBB   | 82     |                  |
| 13  | RAA   | 102    |                  |
| 13  | SAA   | 102    |                  |
| 14  | KOO   | 104    |                  |
| 14  | LOO   | 104    |                  |
| 15  | KPP   | 89     |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 15  | LPP   | 89     |    |
| 16  | KJJ   | 92     |    |
| 16  | LJJ   | 92     |    |
| 17  | LA0   | 246    |    |
| 17  | LA02  | 246    |    |
| 18  | KAA   | 147    |    |
| 18  | LAA   | 147    |    |
| 19  | KB0   | 392    |    |
| 19  | LB0   | 392    |    |
| 20  | KC0   | 328    |   |
| 20  | LC0   | 328    |  |
| 21  | KCC   | 110    |  |
| 21  | LCC   | 110    |  |
| 22  | KDD   | 110    |  |
| 22  | LDD   | 110    |  |
| 23  | KE0   | 171    |  |
| 23  | LE0   | 171    |  |
| 24  | KEE   | 139    |  |
| 24  | LEE   | 139    |  |
| 25  | KF0   | 235    |  |
| 25  | LF0   | 235    |  |
| 26  | KFF   | 111    |  |
| 26  | LFF   | 111    |  |
| 27  | KG0   | 206    |  |
| 27  | LG0   | 206    |  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 28  | KH0   | 187    | 12%<br>97%<br>..  |
| 28  | LH0   | 187    | 11%<br>97%<br>..  |
| 29  | KHH   | 119    | 9%<br>98%<br>..   |
| 29  | LHH   | 119    | 8%<br>98%<br>..   |
| 30  | KI0   | 218    | 11%<br>100%       |
| 30  | LI0   | 218    | 6%<br>100%        |
| 31  | KII   | 98     | 22%<br>98%<br>..  |
| 31  | LII   | 98     | 15%<br>98%<br>..  |
| 32  | KJ0   | 171    | 12%<br>96%<br>..  |
| 32  | LJ0   | 171    | 9%<br>96%<br>..   |
| 33  | KL0   | 165    | 12%<br>96%<br>... |
| 33  | LL0   | 165    | 8%<br>96%<br>...  |
| 34  | KLL   | 52     | 98%<br>.          |
| 34  | LLL   | 52     | 98%<br>.          |
| 35  | KM0   | 122    | 22%<br>93%<br>6%  |
| 35  | LM0   | 122    | 18%<br>93%<br>6%  |
| 36  | KN0   | 204    | 100%              |
| 36  | LN0   | 204    | 100%              |
| 37  | KO0   | 198    | 15%<br>99%<br>.   |
| 37  | LO0   | 198    | 11%<br>99%<br>.   |
| 38  | KP0   | 167    | 6%<br>92%<br>8%   |
| 38  | LP0   | 167    | 7%<br>92%<br>8%   |
| 39  | KQ0   | 183    | 13%<br>99%<br>..  |
| 39  | LQ0   | 183    | 12%<br>99%<br>..  |
| 40  | KR0   | 168    | 15%<br>98%<br>.   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | LR0   | 168    |                  |
| 41  | KS0   | 171    |                  |
| 41  | LS0   | 171    |                  |
| 42  | KT0   | 158    |                  |
| 42  | LT0   | 158    |                  |
| 43  | KU0   | 113    |                  |
| 43  | LU0   | 113    |                  |
| 44  | KV0   | 142    |                  |
| 44  | LV0   | 142    |                  |
| 45  | KW0   | 131    |                  |
| 45  | LW0   | 131    |                  |
| 46  | KX0   | 113    |                  |
| 46  | LX0   | 113    |                  |
| 47  | KY0   | 131    |                  |
| 47  | LY0   | 131    |                  |
| 48  | KZ0   | 153    |                  |
| 48  | LZ0   | 153    |                  |
| 49  | MD1   | 151    |                  |
| 49  | ND1   | 151    |                  |
| 50  | RA0   | 233    |                  |
| 50  | SA0   | 233    |                  |
| 51  | RCC   | 65     |                  |
| 51  | SCC   | 65     |                  |
| 52  | RE0   | 280    |                  |
| 52  | SE0   | 280    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | REE   | 60     |                  |
| 53  | SEE   | 60     |                  |
| 54  | RGG   | 326    |                  |
| 54  | SGG   | 326    |                  |
| 55  | RI0   | 173    |                  |
| 55  | SI0   | 173    |                  |
| 56  | RJ0   | 184    |                  |
| 56  | SJ0   | 184    |                  |
| 57  | RK0   | 107    |                  |
| 57  | SK0   | 107    |                  |
| 58  | RL0   | 155    |                  |
| 58  | SL0   | 155    |                  |
| 59  | RM0   | 130    |                  |
| 59  | SM0   | 130    |                  |
| 60  | RN0   | 143    |                  |
| 60  | SN0   | 143    |                  |
| 61  | RO0   | 135    |                  |
| 61  | SO0   | 135    |                  |
| 62  | RP0   | 163    |                  |
| 62  | SP0   | 163    |                  |
| 63  | RQ0   | 143    |                  |
| 63  | SQ0   | 143    |                  |
| 64  | RR0   | 120    |                  |
| 64  | SR0   | 120    |                  |
| 65  | RS0   | 160    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 65  | SS0   | 160    |                  |
| 66  | RT0   | 143    |                  |
| 66  | ST0   | 143    |                  |
| 67  | RU0   | 119    |                  |
| 67  | SU0   | 119    |                  |
| 68  | RV0   | 67     |                  |
| 68  | SV0   | 67     |                  |
| 69  | RX0   | 141    |                  |
| 69  | SX0   | 141    |                  |
| 70  | RY0   | 146    |                  |
| 70  | SY0   | 146    |                  |
| 71  | RZ0   | 128    |                  |
| 71  | SZ0   | 128    |                  |
| 72  | KD0   | 291    |                  |
| 72  | LD0   | 291    |                  |
| 73  | RDD   | 65     |                  |
| 73  | SDD   | 65     |                  |
| 74  | RD0   | 242    |                  |
| 74  | SD0   | 242    |                  |
| 75  | RG0   | 230    |                  |
| 75  | SG0   | 230    |                  |
| 76  | RH0   | 164    |                  |
| 76  | SH0   | 164    |                  |
| 77  | RW0   | 128    |                  |
| 77  | SW0   | 128    |                  |

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| Mol | Chain | Length | Quality of chain                                                                       |
|-----|-------|--------|----------------------------------------------------------------------------------------|
| 78  | RF0   | 195    | <div><div>8%</div><div><div></div><div>97%</div><div></div></div><div>..</div></div>   |
| 78  | SF0   | 195    | <div><div>9%</div><div><div></div><div>97%</div><div></div></div><div>..</div></div>   |
| 79  | RFF   | 150    | <div><div>18%</div><div><div></div><div>36%</div><div></div></div><div>64%</div></div> |
| 79  | SFF   | 150    | <div><div>17%</div><div><div></div><div>36%</div><div></div></div><div>64%</div></div> |

## 2 Entry composition

There are 80 unique types of molecules in this entry. The entry contains 371532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA 23S.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | K50   | 2605     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 55952 | 24974 | 10318 | 18055 | 2605 |         |       |
| 1   | L50   | 2605     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 55952 | 24974 | 10318 | 18055 | 2605 |         |       |

- Molecule 2 is a RNA chain called RNA 16S.

| Mol | Chain | Residues | Atoms |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 2   | R60   | 1354     | Total | C     | N    | O    | P    | 0       | 0     |
|     |       |          | 29180 | 13024 | 5463 | 9339 | 1354 |         |       |
| 2   | S60   | 1354     | Total | C     | N    | O    | P    | 0       | 0     |
|     |       |          | 29180 | 13024 | 5463 | 9339 | 1354 |         |       |

- Molecule 3 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | E     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1224  | 769 | 218 | 231 | 6 |         |       |
| 3   | D     | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1224  | 769 | 218 | 231 | 6 |         |       |

- Molecule 4 is a protein called Ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | KGG   | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 819   | 504 | 169 | 139 | 7 |         |       |
| 4   | LGG   | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 819   | 504 | 169 | 139 | 7 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | RB0   | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1609  | 1018 | 286 | 298 | 7 |         |       |
| 5   | SB0   | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1609  | 1018 | 286 | 298 | 7 |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | RC0   | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1729  | 1101 | 300 | 321 | 7 |         |       |
| 6   | SC0   | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1729  | 1101 | 300 | 321 | 7 |         |       |

- Molecule 7 is a RNA chain called RNA 5S.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 7   | K70   | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2541  | 1136 | 459 | 827 | 119 |         |       |
| 7   | L70   | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2541  | 1136 | 459 | 827 | 119 |         |       |

- Molecule 8 is a protein called Elongation factor 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 8   | B     | 847      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6606  | 4175 | 1125 | 1264 | 42 |         |       |
| 8   | A     | 847      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6606  | 4175 | 1125 | 1264 | 42 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L10a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | K     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1109 | 291 | 312 | 6 |         |       |
| 9   | L     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1109 | 291 | 312 | 6 |         |       |

- Molecule 10 is a protein called Large ribosomal subunit protein uL10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | N     | 269      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2113  | 1348 | 345 | 407 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | M     | 269      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2113  | 1348 | 345 | 407 | 13 |         |       |

- Molecule 11 is a protein called Ubiquitin.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | KMM   | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 264 | 89 | 70 | 4 |         |       |
| 11  | LMM   | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 264 | 89 | 70 | 4 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | RBB   | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 627   | 394 | 108 | 116 | 9 |         |       |
| 12  | SBB   | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 627   | 394 | 108 | 116 | 9 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | RAA   | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 513 | 163 | 145 | 6 |         |       |
| 13  | SAA   | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 513 | 163 | 145 | 6 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L44.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | KOO   | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 801   | 504 | 163 | 130 | 4 |         |       |
| 14  | LOO   | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 801   | 504 | 163 | 130 | 4 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L37a..

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15  | KPP   | 87       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 684   | 427 | 131 | 116 | 10 |         |       |
| 15  | LPP   | 87       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 684   | 427 | 131 | 116 | 10 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 16  | KJJ   | 89       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 701   | 427 | 146 | 118 | 10 |         |       |
| 16  | LJJ   | 89       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 701   | 427 | 146 | 118 | 10 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | LA0   | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1889  | 1189 | 361 | 334 | 5 |         |       |
| 17  | LA02  | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1889  | 1189 | 361 | 334 | 5 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | KAA   | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1167  | 738 | 229 | 194 | 6 |         |       |
| 18  | LAA   | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1167  | 738 | 229 | 194 | 6 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | KB0   | 383      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3039  | 1926 | 559 | 543 | 11 |         |       |
| 19  | LB0   | 383      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3039  | 1926 | 559 | 543 | 11 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | KC0   | 327      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2604  | 1629 | 478 | 485 | 12 |         |       |
| 20  | LC0   | 327      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2604  | 1629 | 478 | 485 | 12 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | KCC   | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 781   | 504 | 126 | 148 | 3 |         |       |
| 21  | LCC   | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 781   | 504 | 126 | 148 | 3 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | KDD   | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 895   | 575 | 163 | 154 | 3 |         |       |
| 22  | LDD   | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 895   | 575 | 163 | 154 | 3 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | KE0   | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1371  | 879 | 227 | 262 | 3 |         |       |
| 23  | LE0   | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1371  | 879 | 227 | 262 | 3 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | KEE   | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1090  | 697 | 205 | 182 | 6 |         |       |
| 24  | LEE   | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1090  | 697 | 205 | 182 | 6 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25  | KF0   | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1933  | 1234 | 342 | 350 | 7 |         |       |
| 25  | LF0   | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1933  | 1234 | 342 | 350 | 7 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | KFF   | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 893   | 567 | 159 | 162 | 5 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LFF   | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 893   | 567 | 159 | 162 | 5 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27  | KG0   | 199      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1590  | 1015 | 275 | 290 | 10 |         |       |
| 27  | LG0   | 199      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1590  | 1015 | 275 | 290 | 10 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | KH0   | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 951 | 252 | 266 | 8 |         |       |
| 28  | LH0   | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 951 | 252 | 266 | 8 |         |       |

- Molecule 29 is a protein called 60S Ribosomal L29 protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | KHH   | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 993   | 626 | 188 | 176 | 3 |         |       |
| 29  | LHH   | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 993   | 626 | 188 | 176 | 3 |         |       |

- Molecule 30 is a protein called S60 ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 30  | KI0   | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1750  | 1096 | 333 | 308 | 13 |         |       |
| 30  | LI0   | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1750  | 1096 | 333 | 308 | 13 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | KII   | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 496 | 146 | 136 | 6 |         |       |
| 31  | LII   | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 496 | 146 | 136 | 6 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | KJ0   | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1332  | 847 | 242 | 236 | 7 |         |       |
| 32  | LJ0   | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1332  | 847 | 242 | 236 | 7 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 33  | KL0   | 164      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1353  | 857 | 252 | 232 | 12 |         |       |
| 33  | LL0   | 164      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1353  | 857 | 252 | 232 | 12 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | KLL   | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 272 | 87 | 65 | 3 |         |       |
| 34  | LLL   | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 272 | 87 | 65 | 3 |         |       |

- Molecule 35 is a protein called eL14 LM0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | KM0   | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 927   | 588 | 151 | 183 | 5 |         |       |
| 35  | LM0   | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 927   | 588 | 151 | 183 | 5 |         |       |

- Molecule 36 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36  | KN0   | 203      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1688  | 1055 | 346 | 276 | 11 |         |       |
| 36  | LN0   | 203      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1688  | 1055 | 346 | 276 | 11 |         |       |

- Molecule 37 is a protein called Ribosomal protein L13A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37  | KO0   | 198      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1598  | 1018 | 286 | 280 | 14 |         |       |
| 37  | LO0   | 198      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1598  | 1018 | 286 | 280 | 14 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | KP0   | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1238  | 794 | 225 | 213 | 6 |         |       |
| 38  | LP0   | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1238  | 794 | 225 | 213 | 6 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | KQ0   | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1491  | 950 | 270 | 266 | 5 |         |       |
| 39  | LQ0   | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1491  | 950 | 270 | 266 | 5 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | KR0   | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1336  | 832 | 261 | 236 | 7 |         |       |
| 40  | LR0   | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1336  | 832 | 261 | 236 | 7 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | KS0   | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1400  | 898 | 241 | 256 | 5 |         |       |
| 41  | LS0   | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1400  | 898 | 241 | 256 | 5 |         |       |

- Molecule 42 is a protein called 60s ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | KT0   | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1270  | 808 | 233 | 224 | 5 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | LT0   | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1270  | 808 | 233 | 224 | 5 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | KU0   | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 526 | 135 | 147 | 2 |         |       |
| 43  | LU0   | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 526 | 135 | 147 | 2 |         |       |

- Molecule 44 is a protein called Ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | KV0   | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1057  | 663 | 200 | 189 | 5 |         |       |
| 44  | LV0   | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1057  | 663 | 200 | 189 | 5 |         |       |

- Molecule 45 is a protein called Ribosomal protein L24E.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | KW0   | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 539 | 143 | 147 | 3 |         |       |
| 45  | LW0   | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 539 | 143 | 147 | 3 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | KX0   | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 874   | 562 | 156 | 155 | 1 |         |       |
| 46  | LX0   | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 874   | 562 | 156 | 155 | 1 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | KY0   | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1048  | 658 | 197 | 186 | 7 |         |       |
| 47  | LY0   | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1048  | 658 | 197 | 186 | 7 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | KZ0   | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 963   | 618 | 172 | 169 | 4 |         |       |
| 48  | LZ0   | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 963   | 618 | 172 | 169 | 4 |         |       |

- Molecule 49 is a protein called DNL-type domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 49  | ND1   | 151      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1229  | 776 | 201 | 241 | 11 |         |       |
| 49  | MD1   | 151      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1229  | 776 | 201 | 241 | 11 |         |       |

- Molecule 50 is a protein called 40S ribosomal protein S0.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | RA0   | 220      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1725  | 1091 | 292 | 328 | 14 |         |       |
| 50  | SA0   | 220      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1725  | 1091 | 292 | 328 | 14 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51  | RCC   | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 295 | 86 | 91 | 4 |         |       |
| 51  | SCC   | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 295 | 86 | 91 | 4 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | RE0   | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2044  | 1297 | 361 | 379 | 7 |         |       |
| 52  | SE0   | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2044  | 1297 | 361 | 379 | 7 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 53  | REE   | 56       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 447   | 284 | 89 | 74 |         |       |
| 53  | SEE   | 56       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 447   | 284 | 89 | 74 |         |       |

- Molecule 54 is a protein called Guanine nucleotide binding protein beta subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 54  | RGG   | 319      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2478  | 1558 | 411 | 494 | 15 |         |       |
| 54  | SGG   | 319      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2478  | 1558 | 411 | 494 | 15 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | RI0   | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1347  | 834 | 266 | 240 | 7 |         |       |
| 55  | SI0   | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1347  | 834 | 266 | 240 | 7 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | RJ0   | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1379  | 880 | 252 | 243 | 4 |         |       |
| 56  | SJ0   | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1379  | 880 | 252 | 243 | 4 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | RK0   | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 737   | 472 | 127 | 135 | 3 |         |       |
| 57  | SK0   | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 737   | 472 | 127 | 135 | 3 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | RL0   | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1229  | 790 | 217 | 216 | 6 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | SL0   | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1229  | 790 | 217 | 216 | 6 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | RM0   | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 553 | 156 | 162 | 5 |         |       |
| 59  | SM0   | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 553 | 156 | 162 | 5 |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | RN0   | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1130  | 728 | 196 | 202 | 4 |         |       |
| 60  | SN0   | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1130  | 728 | 196 | 202 | 4 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | RO0   | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 983   | 606 | 191 | 183 | 3 |         |       |
| 61  | SO0   | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 983   | 606 | 191 | 183 | 3 |         |       |

- Molecule 62 is a protein called Ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | RP0   | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 598 | 172 | 173 | 7 |         |       |
| 62  | SP0   | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 598 | 172 | 173 | 7 |         |       |

- Molecule 63 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | RQ0   | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 726 | 204 | 207 | 6 |         |       |
| 63  | SQ0   | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 726 | 204 | 207 | 6 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | RR0   | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 974   | 613 | 172 | 186 | 3 |         |       |
| 64  | SR0   | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 974   | 613 | 172 | 186 | 3 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | RS0   | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1150  | 720 | 220 | 207 | 3 |         |       |
| 65  | SS0   | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1150  | 720 | 220 | 207 | 3 |         |       |

- Molecule 66 is a protein called 40S Ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | RT0   | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1161  | 741 | 208 | 211 | 1 |         |       |
| 66  | ST0   | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1161  | 741 | 208 | 211 | 1 |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | RU0   | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 809   | 515 | 144 | 143 | 7 |         |       |
| 67  | SU0   | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 809   | 515 | 144 | 143 | 7 |         |       |

- Molecule 68 is a protein called Ribosomal protein S21E.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 68  | RV0   | 65       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 521   | 319 | 96 | 101 | 5 |         |       |
| 68  | SV0   | 65       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 521   | 319 | 96 | 101 | 5 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | RX0   | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 692 | 216 | 186 | 4 |         |       |
| 69  | SX0   | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 692 | 216 | 186 | 4 |         |       |

- Molecule 70 is a protein called 40s ribosomal protein s24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | RY0   | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1118  | 693 | 215 | 204 | 6 |         |       |
| 70  | SY0   | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1118  | 693 | 215 | 204 | 6 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | RZ0   | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 633   | 403 | 116 | 113 | 1 |         |       |
| 71  | SZ0   | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 633   | 403 | 116 | 113 | 1 |         |       |

- Molecule 72 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 72  | KD0   | 281      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2298  | 1451 | 410 | 426 | 11 |         |       |
| 72  | LD0   | 281      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2298  | 1451 | 410 | 426 | 11 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 73  | RDD   | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 550   | 345 | 102 | 96 | 7 |         |       |
| 73  | SDD   | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 550   | 345 | 102 | 96 | 7 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 74  | RD0   | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1700  | 1085 | 300 | 307 | 8 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 74  | SD0   | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1700  | 1085 | 300 | 307 | 8 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 75  | RG0   | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1835  | 1178 | 325 | 328 | 4 |         |       |
| 75  | SG0   | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1835  | 1178 | 325 | 328 | 4 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | RH0   | 163      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1335  | 855 | 219 | 255 | 6 |         |       |
| 76  | SH0   | 163      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1335  | 855 | 219 | 255 | 6 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S15A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | RW0   | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 639 | 195 | 180 | 8 |         |       |
| 77  | SW0   | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 639 | 195 | 180 | 8 |         |       |

- Molecule 78 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | RF0   | 192      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1509  | 953 | 275 | 275 | 6 |         |       |
| 78  | SF0   | 192      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1509  | 953 | 275 | 275 | 6 |         |       |

- Molecule 79 is a protein called Ubiquitin/40s ribosomal protein S27a fusion.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 79  | RFF   | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 413   | 256 | 74 | 78 | 5 |         |       |
| 79  | SFF   | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 413   | 256 | 74 | 78 | 5 |         |       |

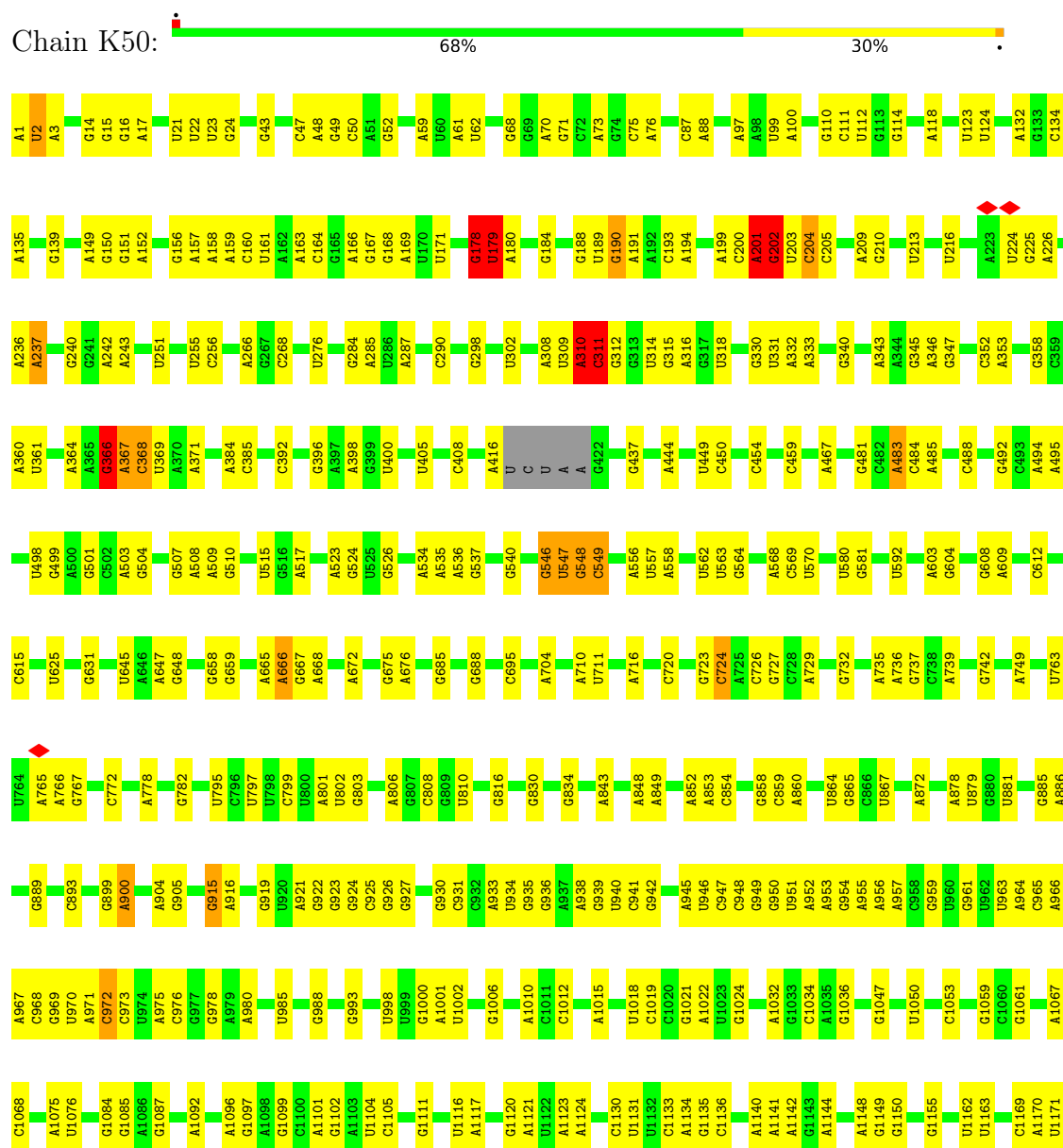
- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 80  | KGG   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | KMM   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | RBB   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | RAA   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | KOO   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | KPP   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | KJJ   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | ND1   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | RFF   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | LGG   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | LMM   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | SBB   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | SAA   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | LOO   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | LPP   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | LJJ   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | MD1   | 1        | Total<br>1 | Zn<br>1 | 0       |
| 80  | SFF   | 1        | Total<br>1 | Zn<br>1 | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: RNA 23S



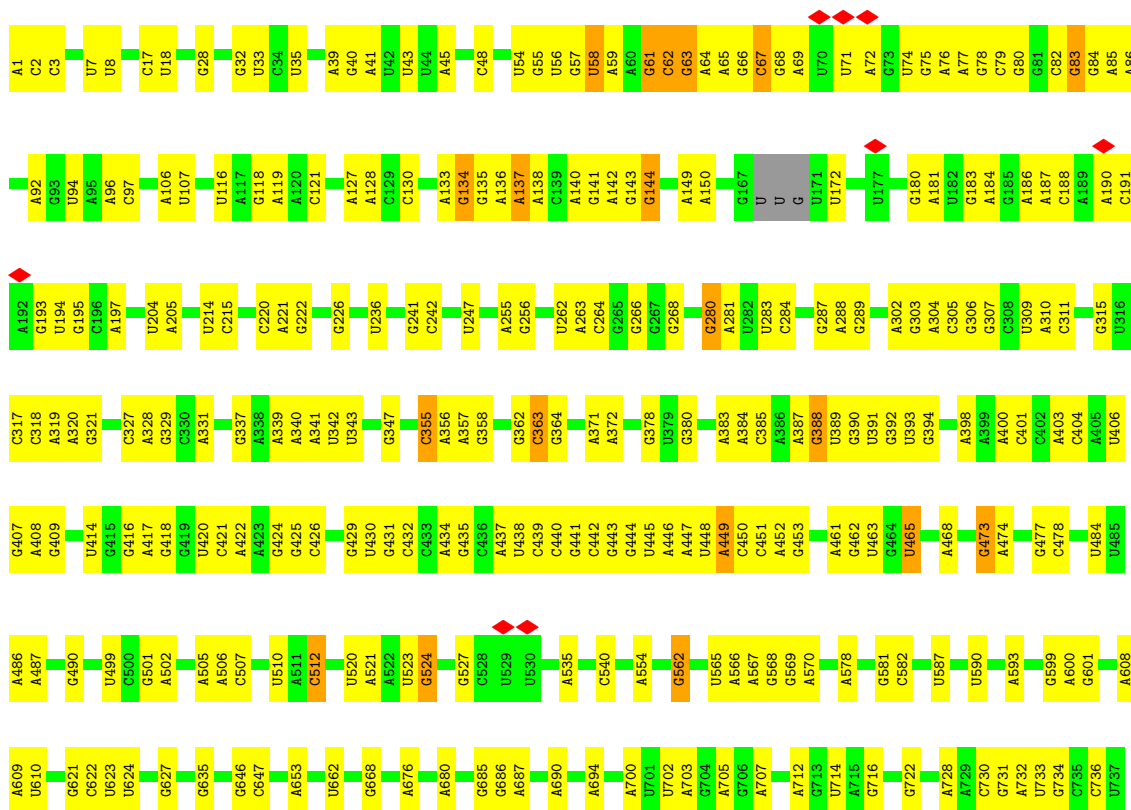


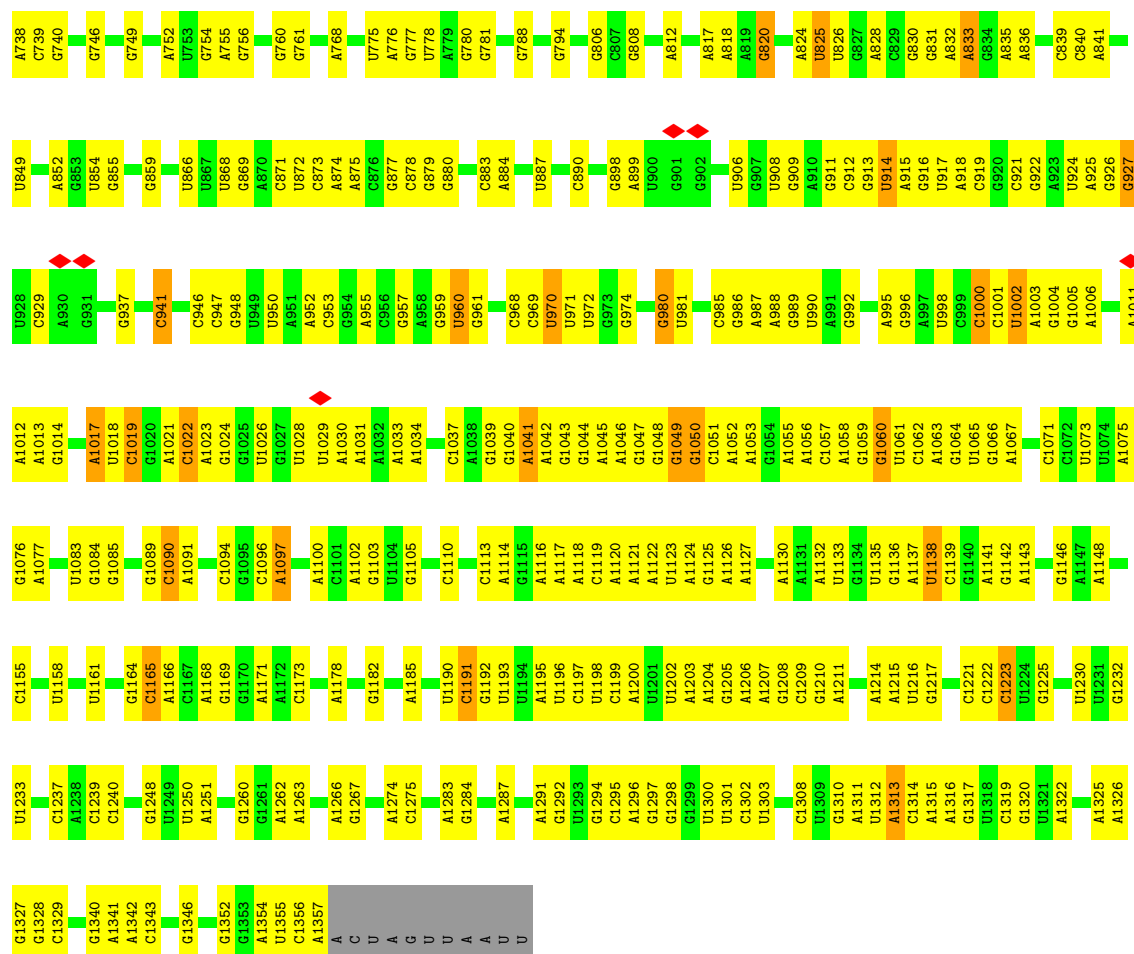
| Frequency | Percentage |
|-----------|------------|
| Often     | 68%        |
| Sometimes | 30%        |



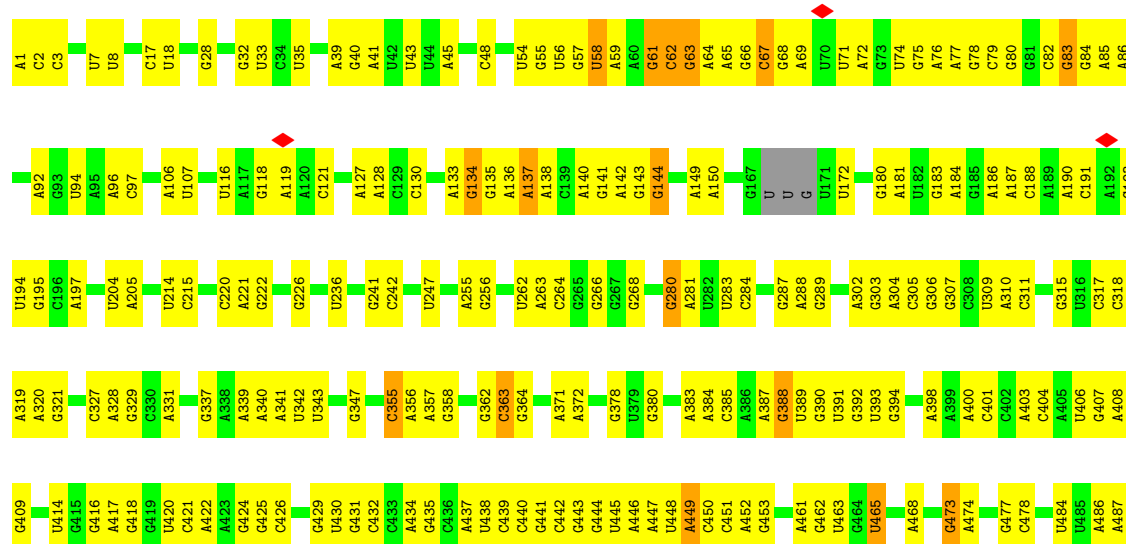
|      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |
|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|
| A135 | A236 | A360 | U498 | C615 | U764 | G889 | A967  | C1068 | A1172 | G1277 | U1430 | U1564 | G1709 | U1846 |
| G139 | A237 | U361 | G499 | U625 | A765 | G889 | C968  | A1076 | A1173 | U1278 | G1431 | U1565 | A1715 | A1854 |
| A149 | G240 | A364 | A500 | G631 | A766 | C893 | U970  | U1076 | A1176 | A1281 | A1437 | A1571 | A1716 | A1854 |
| G150 | A242 | A365 | C502 | G645 | G241 | G899 | C972  | G1084 | G1177 | A1282 | U1441 | G1572 | A1717 | G1862 |
| G151 | A243 | A366 | A503 | A646 | G242 | A900 | C973  | G1085 | G1181 | A1283 | C1442 | G1573 | G1718 | G1862 |
| A152 | U251 | A367 | G504 | G647 | G243 | A904 | U974  | A1086 | G1182 | A1284 | C1443 | G1574 | G1719 | A1869 |
| G156 | U255 | C368 | G507 | G648 | A244 | G905 | C976  | G1087 | G1183 | A1308 | A1449 | A1583 | C1720 | A1875 |
| A157 | C256 | A371 | A508 | G658 | A245 | G915 | G978  | A1092 | C1184 | C1309 | A1450 | U1592 | G1723 | A1876 |
| A158 | A266 | A384 | A509 | G659 | A246 | A916 | A979  | A1096 | U1189 | A1327 | U1454 | C1603 | G1724 | U1880 |
| A159 | G267 | C385 | G510 | A665 | A247 | A919 | A980  | G1097 | C1190 | A1332 | C1457 | G1609 | A1731 | U1881 |
| U161 | G268 | C392 | U515 | A666 | A248 | U920 | U985  | A1098 | U1191 | G1332 | A1458 | G1610 | A1732 | U1882 |
| A163 | C269 | G667 | A517 | G667 | A249 | A921 | U988  | G1099 | A1192 | G1339 | C1459 | A1610 | U1734 | A1883 |
| C164 | U276 | G396 | A523 | A668 | A250 | G922 | G988  | C1100 | G1198 | A1340 | U1463 | G1611 | A1739 | G1884 |
| G165 | G284 | A397 | A524 | A672 | A251 | G923 | G993  | C1101 | G1199 | A1341 | C1464 | G1612 | C1740 | G1885 |
| A166 | A285 | A398 | G525 | G675 | A252 | G924 | G993  | A1102 | G1204 | G1342 | C1465 | A1613 | G1741 | C1886 |
| G167 | A286 | A399 | G526 | A676 | A253 | C925 | U998  | A1103 | G1205 | A1346 | A1466 | G1614 | G1742 | A1887 |
| G168 | U287 | U400 | G526 | A710 | A254 | G926 | U999  | U1104 | G1206 | A1351 | A1467 | G1619 | G1743 | A1889 |
| A169 | U170 | U405 | A534 | A711 | A255 | G927 | U999  | C1105 | A1207 | C1351 | G1468 | U1619 | C1744 | G1890 |
| U171 | C290 | C408 | A535 | A716 | A256 | G930 | G1000 | G1111 | A1217 | C1360 | G1474 | A1625 | A1745 | G1893 |
| G178 | G298 | U416 | A536 | A717 | A257 | C931 | A1001 | U1116 | A1218 | U1360 | A1474 | G1626 | A1746 | G1894 |
| A180 | U302 | A416 | G537 | A718 | A258 | C932 | U1002 | A1117 | A1223 | U1374 | G1485 | U1628 | A1749 | G1895 |
| G184 | A308 | U416 | G540 | A719 | A259 | C933 | G1006 | U1117 | A1224 | G1375 | G1486 | C1629 | U1750 | A1896 |
| U309 | A310 | U416 | G546 | A719 | A260 | U934 | A1010 | G1120 | A1225 | A1383 | A1487 | G1643 | G1751 | G1897 |
| G188 | C311 | U416 | U547 | A720 | A261 | G935 | A1011 | G1121 | A1226 | U1384 | U1488 | G1644 | G1752 | C1898 |
| U189 | G312 | U416 | C549 | A721 | A262 | G936 | C1011 | A1122 | A1227 | G1385 | G1489 | U1645 | A1753 | U1899 |
| G190 | G313 | U416 | G556 | A722 | A263 | G937 | C1012 | A1123 | G1228 | U1386 | U1490 | C1645 | G1754 | A1900 |
| A191 | U314 | U416 | U557 | A723 | A264 | A938 | A1015 | A1124 | U1230 | A1387 | U1491 | G1649 | A1755 | A1901 |
| A192 | G315 | U416 | A558 | A724 | A265 | U940 | U1018 | C1130 | U1231 | G1388 | U1492 | C1650 | G1756 | A1902 |
| C193 | A194 | U416 | U558 | A725 | A266 | C941 | U1131 | U1131 | G1232 | C1388 | G1500 | A1651 | A1760 | G1903 |
| A199 | U318 | U416 | U562 | A726 | A267 | G942 | C1020 | C1133 | A1234 | G1391 | A1503 | G1652 | G1771 | G1905 |
| C200 | G330 | U416 | U563 | A727 | A268 | U945 | G1021 | A1134 | U1235 | G1392 | G1504 | G1653 | U1772 | C1906 |
| A201 | U331 | U416 | C569 | A728 | A269 | U946 | A1022 | G1135 | U1236 | U1393 | G1505 | A1668 | A1797 | G1907 |
| G202 | A332 | U416 | U570 | A729 | A270 | C948 | U1023 | C1136 | U1237 | U1394 | G1506 | A1669 | C1797 | C1908 |
| U203 | A333 | U416 | U570 | A730 | A271 | G949 | G1024 | A1140 | G1247 | U1395 | U1507 | G1675 | A1801 | A1909 |
| C204 | G340 | U416 | U580 | A731 | A272 | U951 | A1032 | A1141 | C1250 | G1396 | G1513 | A1679 | C1802 | A1910 |
| C205 | A343 | U416 | G581 | A732 | A273 | U952 | G1033 | A1142 | C1254 | A1400 | U1527 | A1680 | A1803 | C1912 |
| A209 | G210 | U416 | U582 | A733 | A274 | U953 | C1034 | A1143 | C1254 | C1411 | U1527 | G1685 | A1808 | A1915 |
| G210 | A344 | U416 | U583 | A734 | A275 | U954 | A1035 | A1144 | A1257 | C1412 | G1535 | G1686 | A1809 | A1916 |
| U213 | G345 | U416 | A603 | A735 | A276 | G955 | A1036 | A1145 | A1257 | A1413 | G1536 | G1687 | C1810 | G1917 |
| U216 | A346 | U416 | G604 | A736 | A277 | U956 | G1036 | G1149 | C1264 | U1414 | U1539 | A1688 | G1811 | U1918 |
| A223 | C352 | U416 | G608 | A737 | A278 | U957 | G1047 | G1150 | U1268 | G1415 | A1539 | A1692 | G1828 | G1919 |
| U224 | A353 | U416 | A609 | A738 | A279 | U958 | U1050 | G1155 | U1268 | A1416 | G1547 | C1693 | A1832 | A1920 |
| G225 | G358 | U416 | C612 | A739 | A280 | U959 | C1053 | G1162 | U1269 | U1417 | U1554 | U1700 | A1833 | A1921 |
| A226 | C359 | U416 | U763 | A740 | A281 | U960 | C1053 | U1163 | U1270 | U1417 | G1555 | U1701 | G1835 | G1922 |
|      |      |      |      | A749 | A282 | U961 | G1059 | U1163 | U1271 | A1422 | U1556 | U1702 | A1836 | A1924 |
|      |      |      |      | U763 | A283 | U962 | G1060 | C1169 | A1272 | U1427 | U1557 | A1706 | G1837 | C1925 |
|      |      |      |      |      | A284 | U963 | G1061 | A1170 | C1273 | U1428 | G1557 | A1707 | G1838 | C1926 |
|      |      |      |      |      | A285 | C965 | G1061 | U1171 | C1274 | A1429 | A1563 | A1927 | A1839 | C1928 |
|      |      |      |      |      | A286 | A966 | A1067 |       |       |       |       | U1929 |       | G1930 |

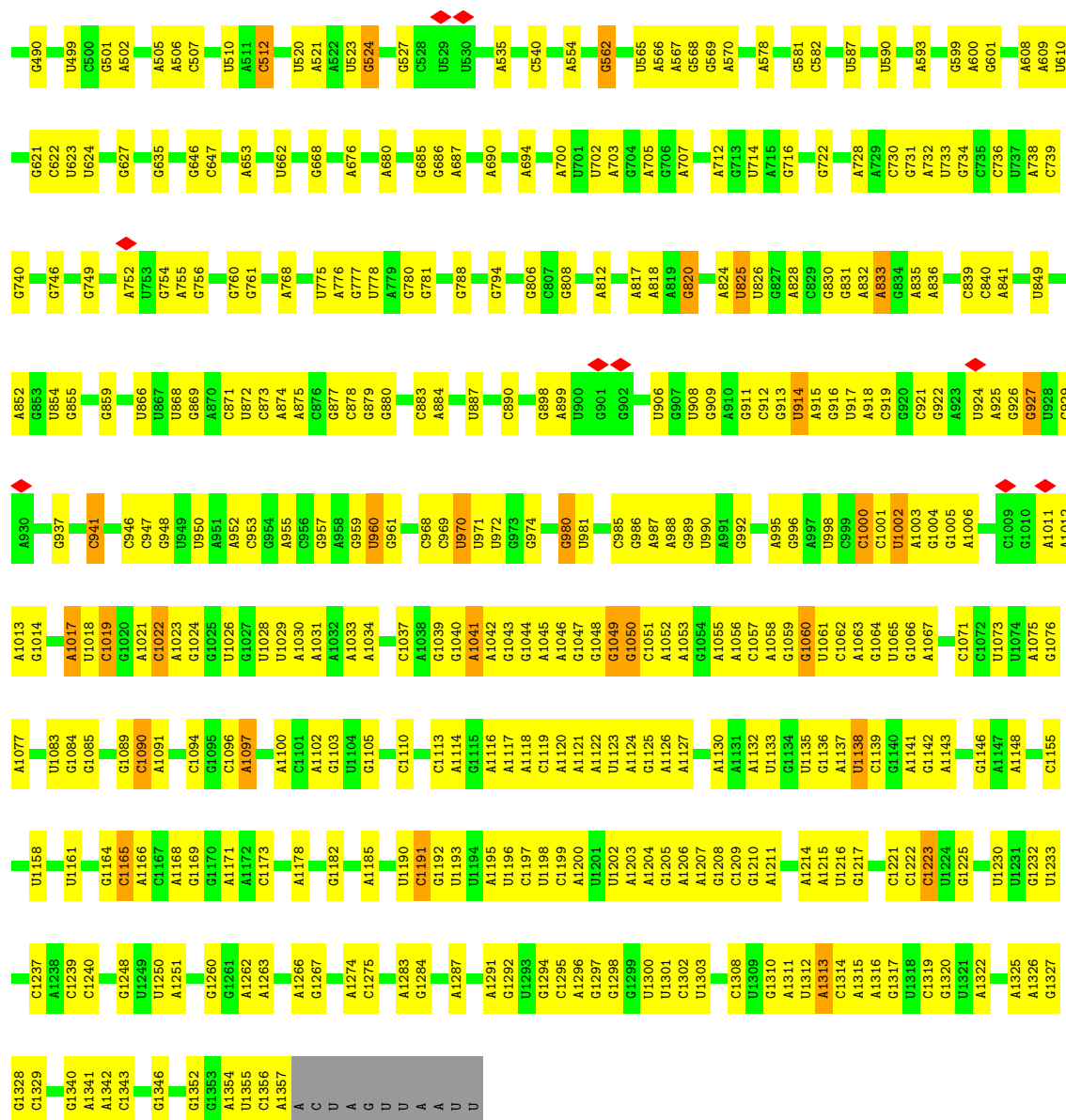
- Molecule 2: RNA 16S



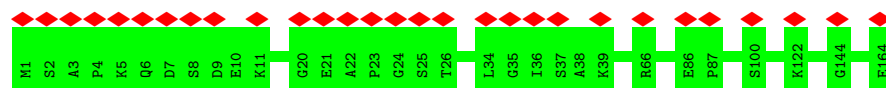


### • Molecule 2: RNA 16S

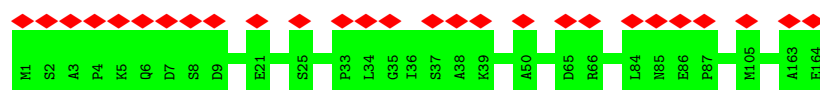




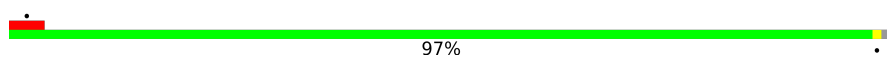
• Molecule 3: 60S ribosomal protein L12

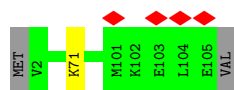


• Molecule 3: 60S ribosomal protein L12

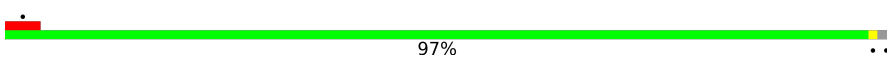


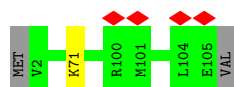
- Molecule 4: Ribosomal protein L34

Chain KGG:  97%

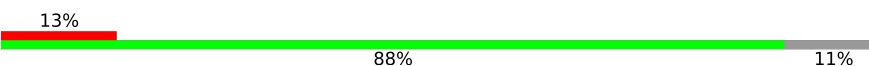


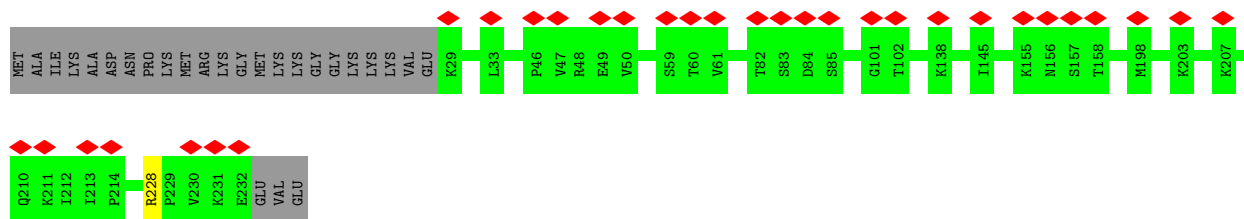
- Molecule 4: Ribosomal protein L34

Chain LGG:  97%

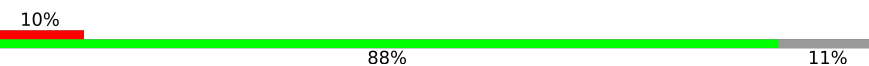


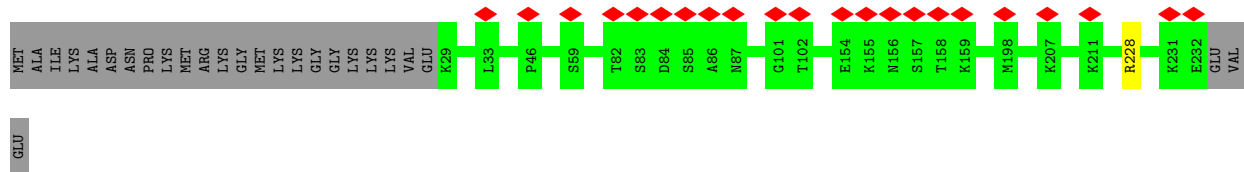
- Molecule 5: 40S ribosomal protein S1

Chain RB0:  13% 88% 11%

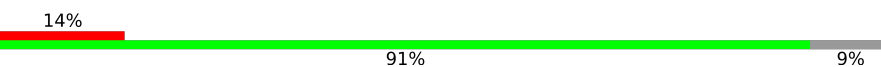


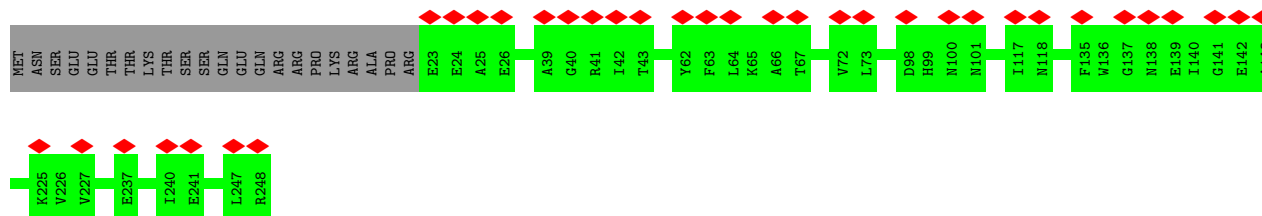
- Molecule 5: 40S ribosomal protein S1

Chain SB0:  10% 88% 11%

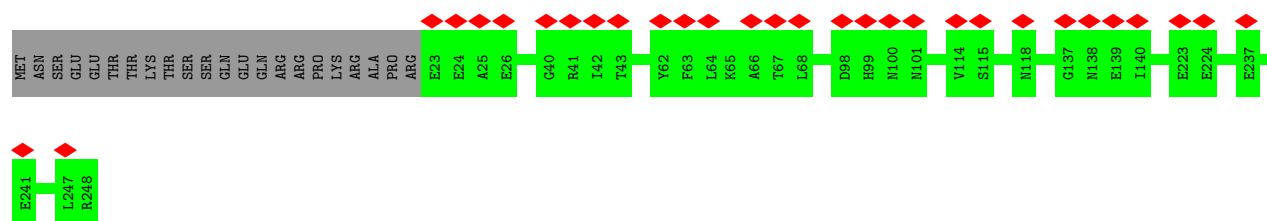


- Molecule 6: 40S ribosomal protein S2

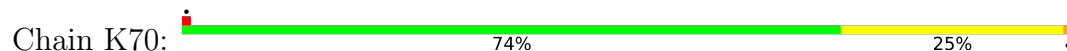
Chain RC0:  14% 91% 9%



- Molecule 6: 40S ribosomal protein S2



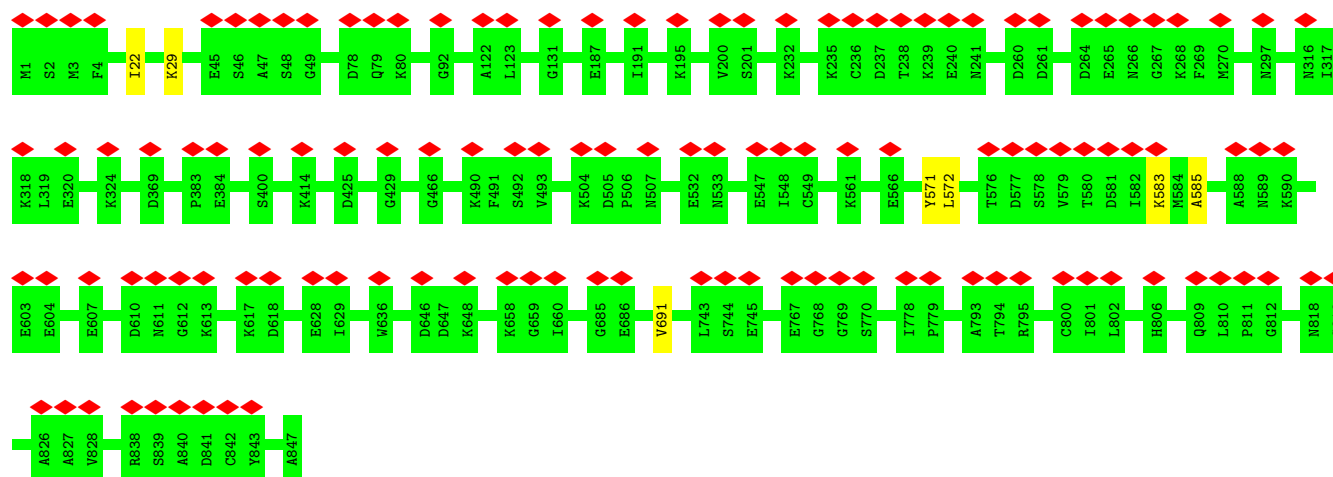
- Molecule 7: RNA 5S



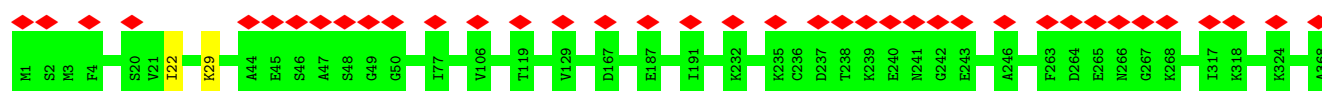
- Molecule 7: RNA 5S

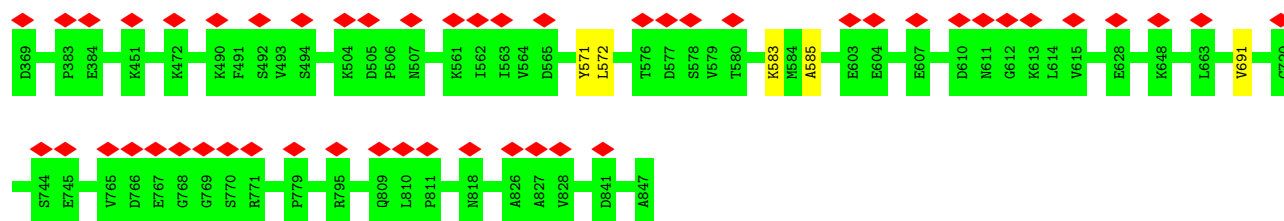


- Molecule 8: Elongation factor 2

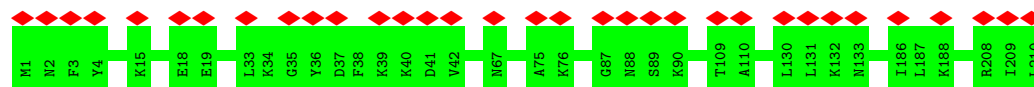


- Molecule 8: Elongation factor 2

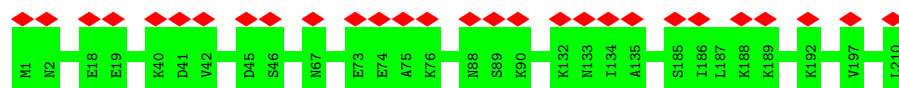




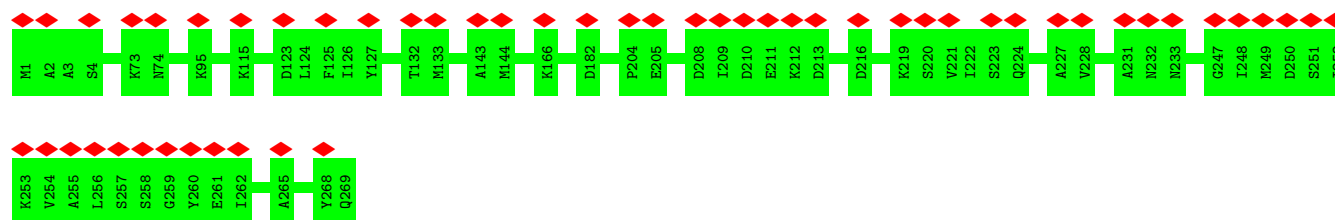
• Molecule 9: 60S ribosomal protein L10a



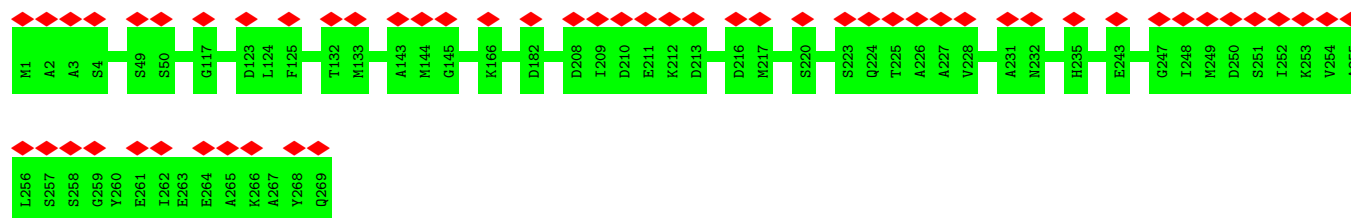
• Molecule 9: 60S ribosomal protein L10a



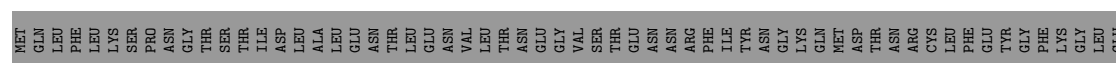
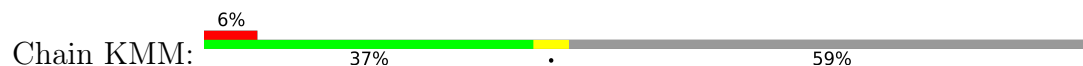
• Molecule 10: Large ribosomal subunit protein uL10



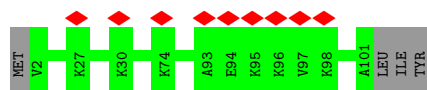
• Molecule 10: Large ribosomal subunit protein uL10



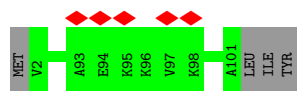
• Molecule 11: Ubiquitin



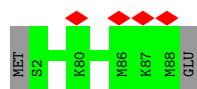




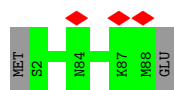
- Molecule 14: 60S ribosomal protein L44



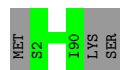
- Molecule 15: 60S ribosomal protein L37a.



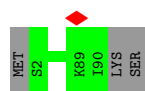
- Molecule 15: 60S ribosomal protein L37a.



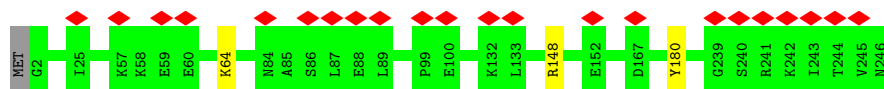
- Molecule 16: 60S ribosomal protein L37



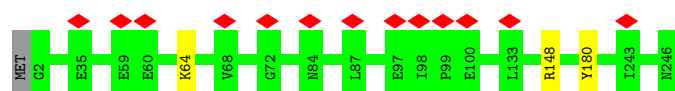
- Molecule 16: 60S ribosomal protein L37



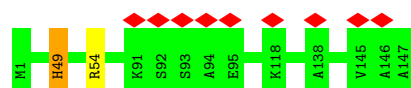
- Molecule 17: 60S ribosomal protein L8



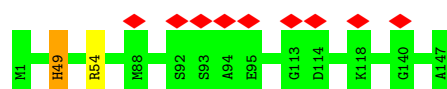
- Molecule 17: 60S ribosomal protein L8



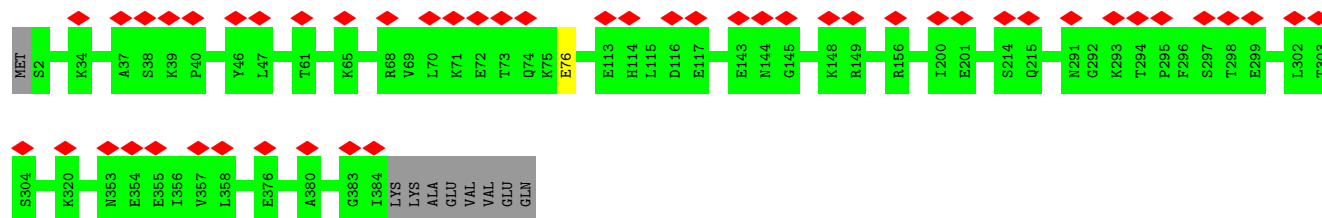
- Molecule 18: 60S ribosomal protein L15



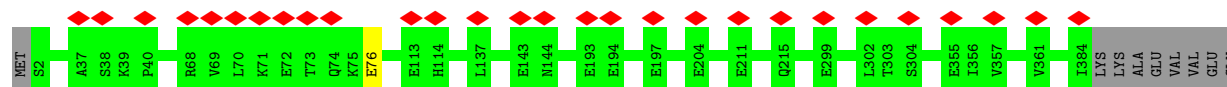
- Molecule 18: 60S ribosomal protein L15



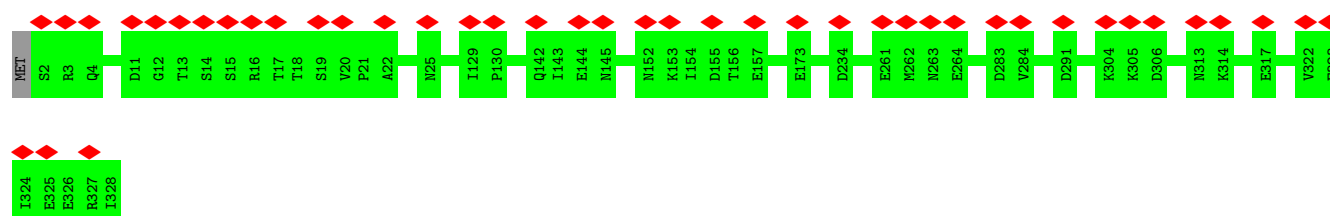
- Molecule 19: 60S ribosomal protein L3



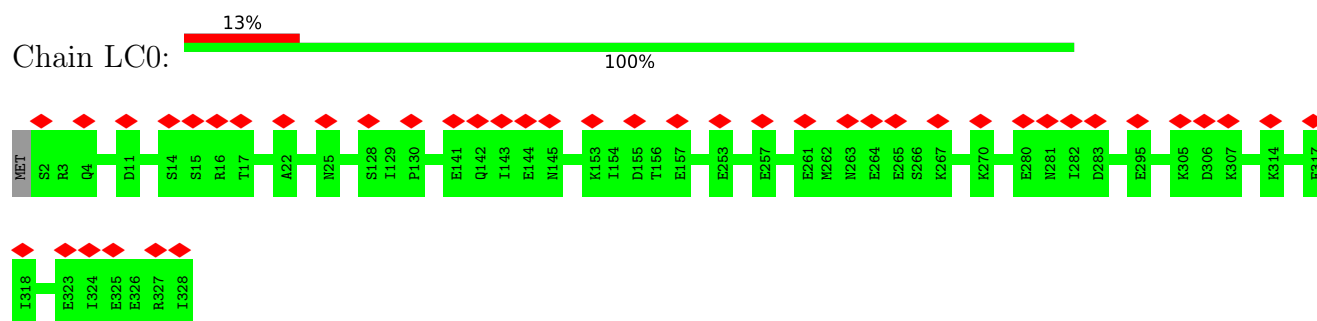
- Molecule 19: 60S ribosomal protein L3



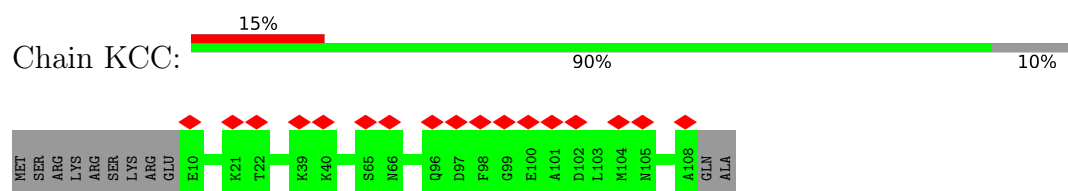
- Molecule 20: 60S ribosomal protein L4



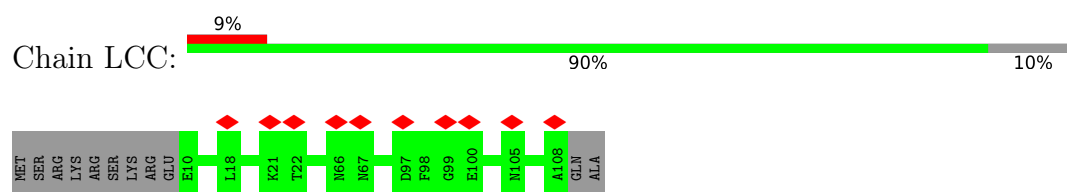
## • Molecule 20: 60S ribosomal protein L4



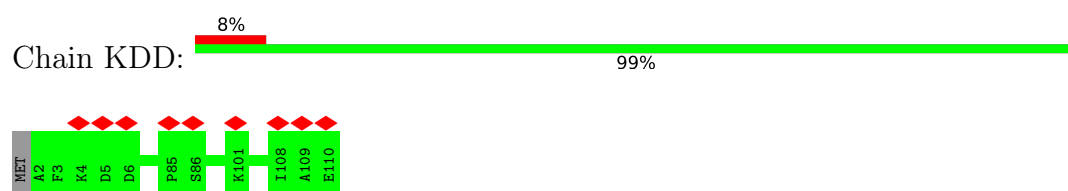
## • Molecule 21: 60S ribosomal protein L3



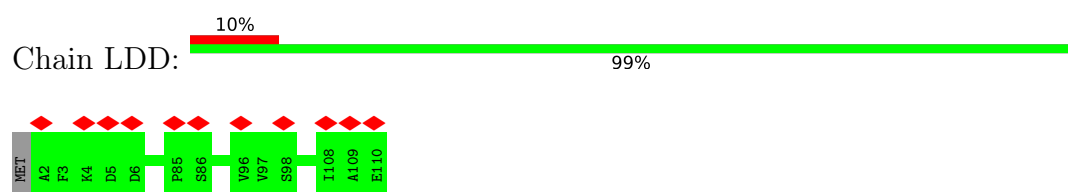
## • Molecule 21: 60S ribosomal protein L3



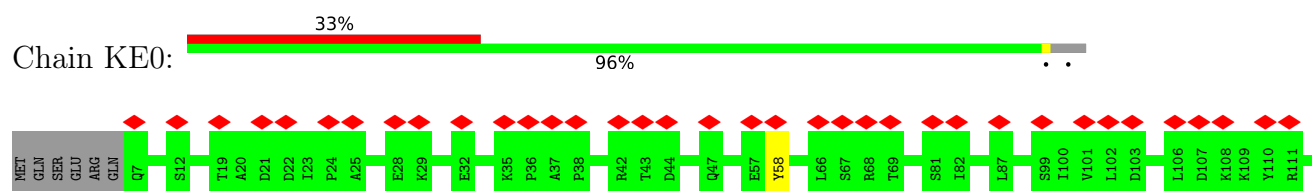
## • Molecule 22: 60S ribosomal protein L31

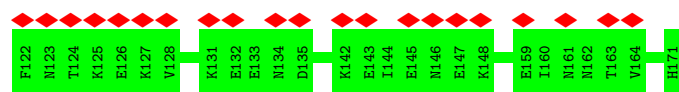


## • Molecule 22: 60S ribosomal protein L31

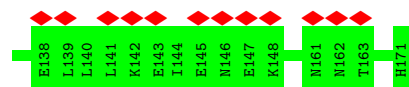
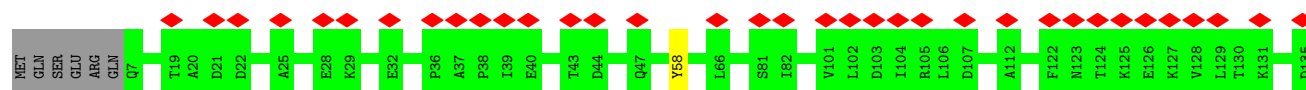


## • Molecule 23: 60S ribosomal protein L6

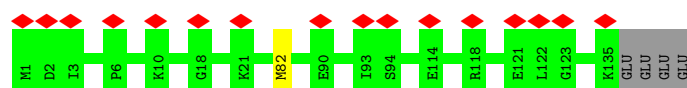




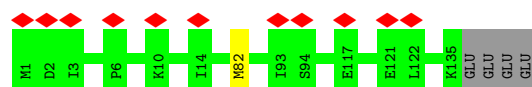
- Molecule 23: 60S ribosomal protein L6



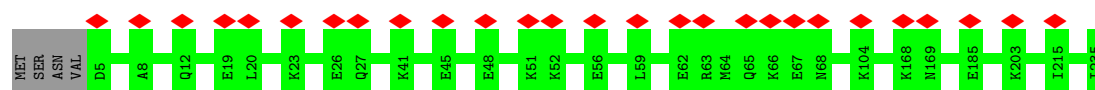
- Molecule 24: 60S ribosomal protein L32



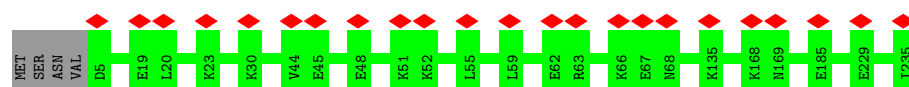
- Molecule 24: 60S ribosomal protein L32



- Molecule 25: 60S ribosomal protein L7

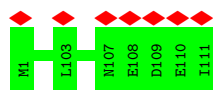


- Molecule 25: 60S ribosomal protein L7

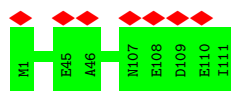


- Molecule 26: 60S ribosomal protein L35a

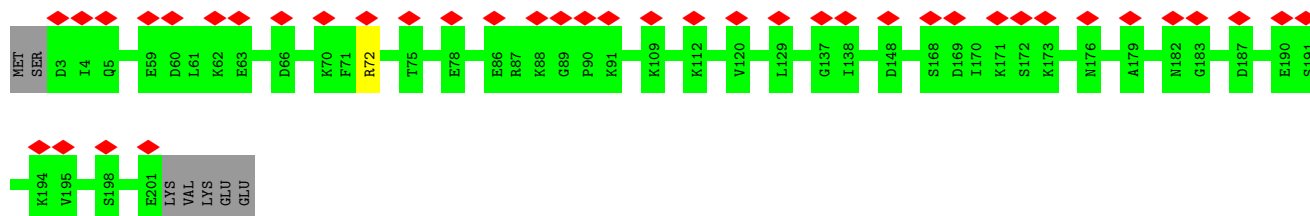




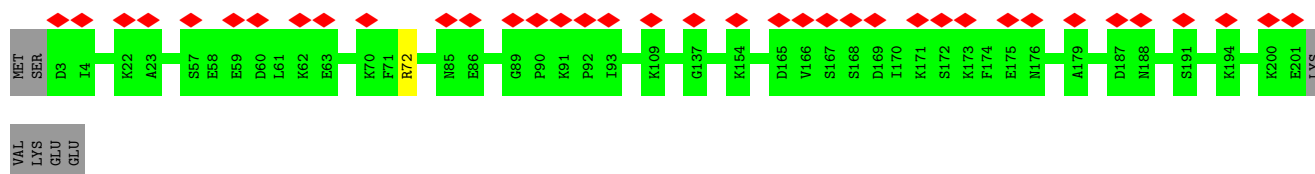
- Molecule 26: 60S ribosomal protein L35a



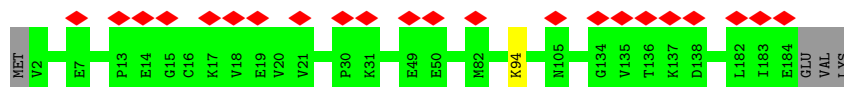
- Molecule 27: 60S ribosomal protein L8



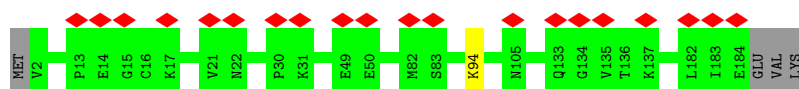
- Molecule 27: 60S ribosomal protein L8



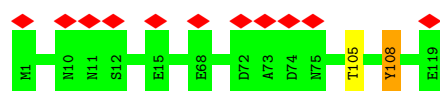
- Molecule 28: 60S ribosomal protein L9



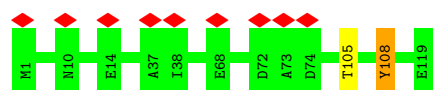
- Molecule 28: 60S ribosomal protein L9



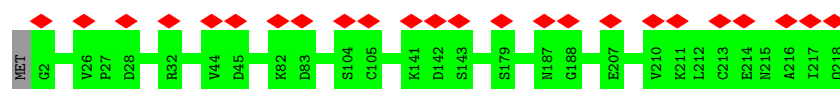
- Molecule 29: 60S Ribosomal L29 protein



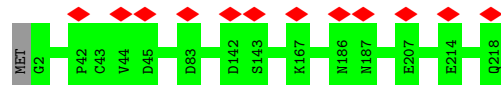
- Molecule 29: 60S Ribosomal L29 protein



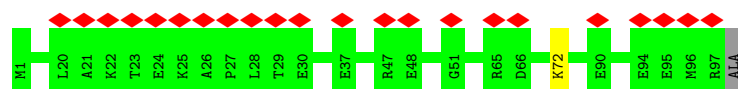
- Molecule 30: S60 ribosomal protein L10



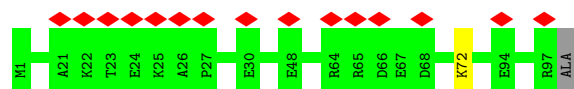
- Molecule 30: S60 ribosomal protein L10



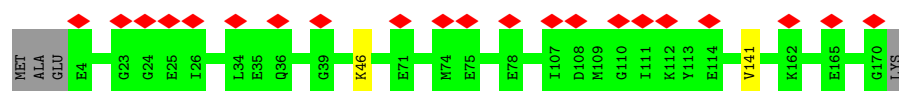
- Molecule 31: 60S ribosomal protein L36



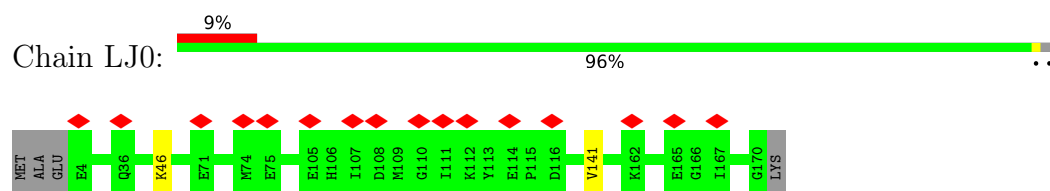
- Molecule 31: 60S ribosomal protein L36



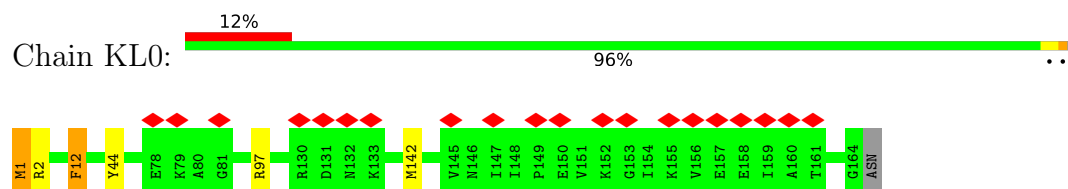
- Molecule 32: 60S ribosomal protein L11



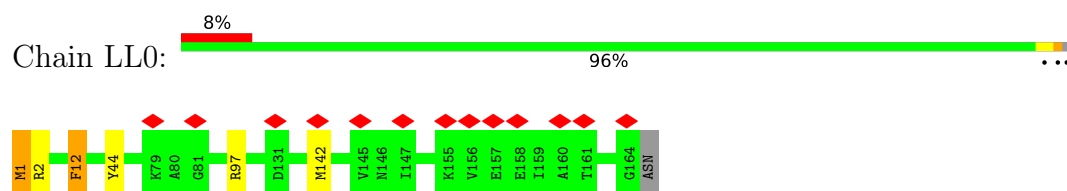
- Molecule 32: 60S ribosomal protein L11



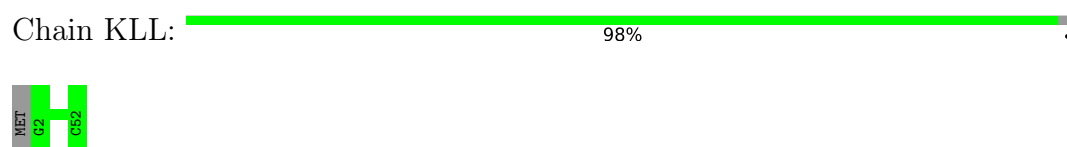
- Molecule 33: 60S ribosomal protein L13



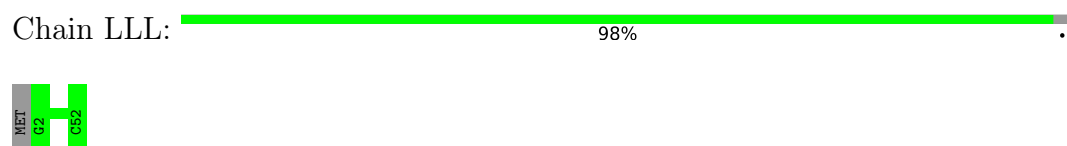
- Molecule 33: 60S ribosomal protein L13



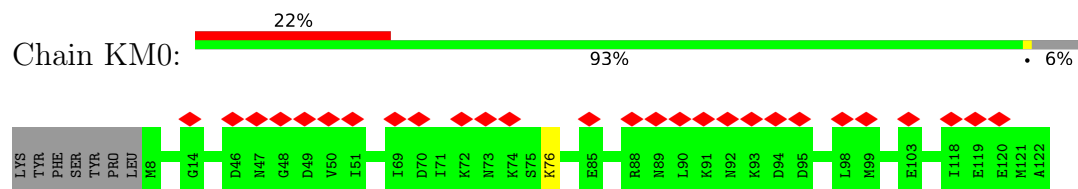
- Molecule 34: 60S ribosomal protein L39



- Molecule 34: 60S ribosomal protein L39

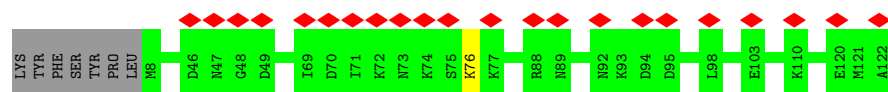


- Molecule 35: eL14 LM0



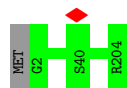
- Molecule 35: eL14 LM0





- Molecule 36: Ribosomal protein L15

Chain KN0: 100%



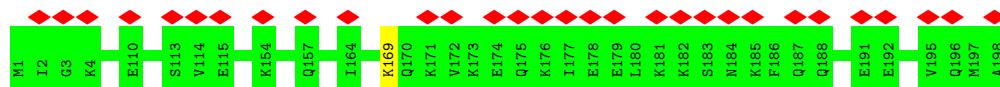
- Molecule 36: Ribosomal protein L15

Chain LN0: 100%



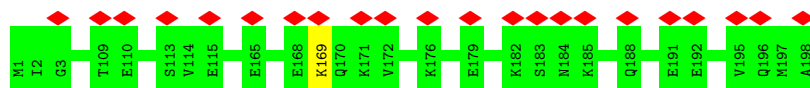
- Molecule 37: Ribosomal protein L13A

Chain KO0: 15% 99%



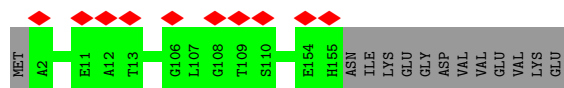
- Molecule 37: Ribosomal protein L13A

Chain LO0: 11% 99%



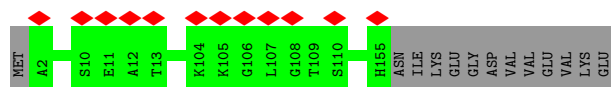
- Molecule 38: 60S ribosomal protein L17

Chain KP0: 6% 92% 8%

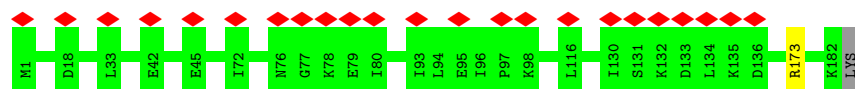


- Molecule 38: 60S ribosomal protein L17

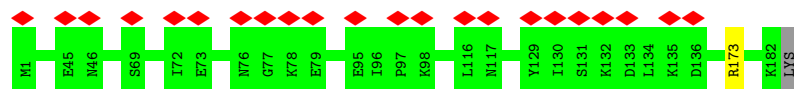
Chain LP0: 7% 92% 8%



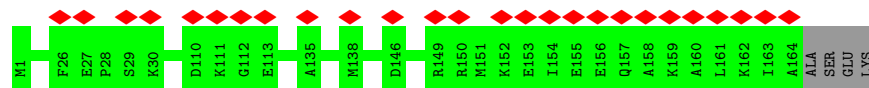
- Molecule 39: 60S ribosomal protein L18



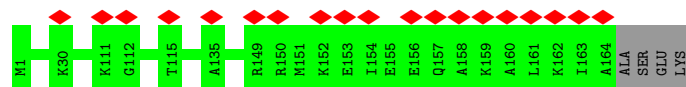
- Molecule 39: 60S ribosomal protein L18



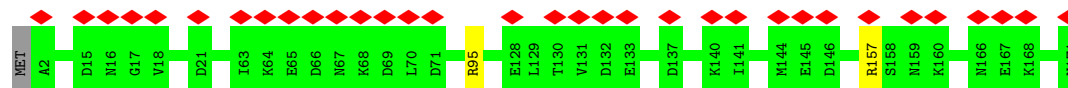
- Molecule 40: 60S ribosomal protein L19



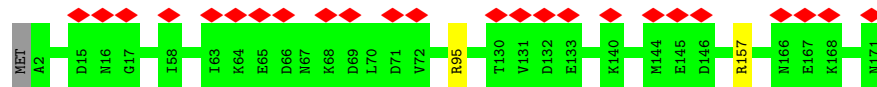
- Molecule 40: 60S ribosomal protein L19



- Molecule 41: 60S ribosomal protein L20

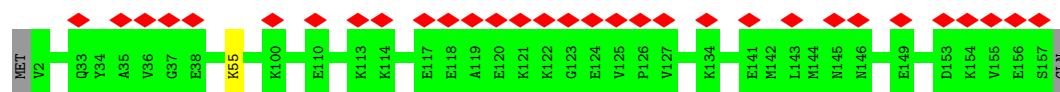


- Molecule 41: 60S ribosomal protein L20

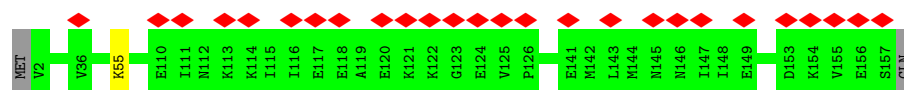


- Molecule 42: 60s ribosomal protein L21

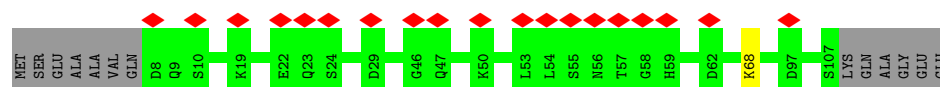




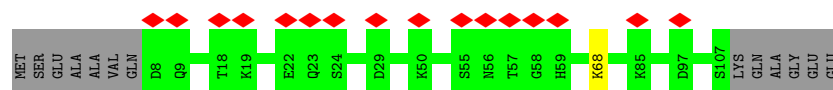
- Molecule 42: 60s ribosomal protein L21



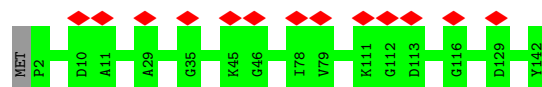
- Molecule 43: 60S ribosomal protein L22



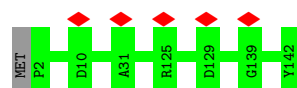
- Molecule 43: 60S ribosomal protein L22



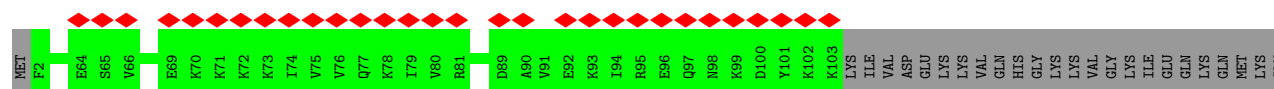
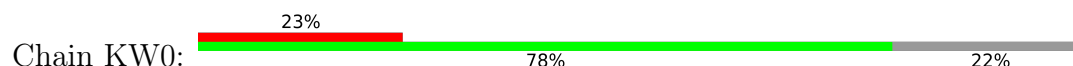
- Molecule 44: Ribosomal protein L23



- Molecule 44: Ribosomal protein L23



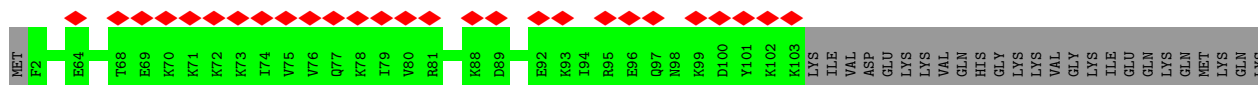
- Molecule 45: Ribosomal protein L24E



LYS  
GLN  
LYS  
TYR

- Molecule 45: Ribosomal protein L24E

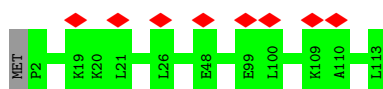
Chain LW0:  21% 78% 22%



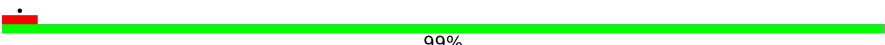
GLN  
LYS  
TYR

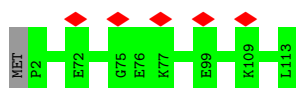
- Molecule 46: 60S ribosomal protein L23a

Chain KX0:  7% 99%



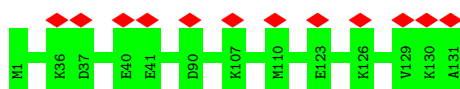
- Molecule 46: 60S ribosomal protein L23a

Chain LX0:  99%



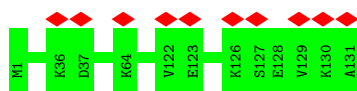
- Molecule 47: 60S ribosomal protein L26

Chain KY0:  9% 100%



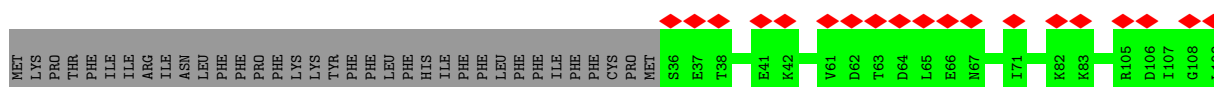
- Molecule 47: 60S ribosomal protein L26

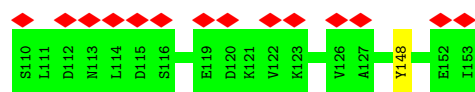
Chain LY0:  8% 100%



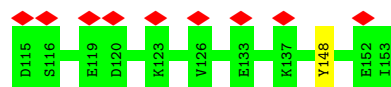
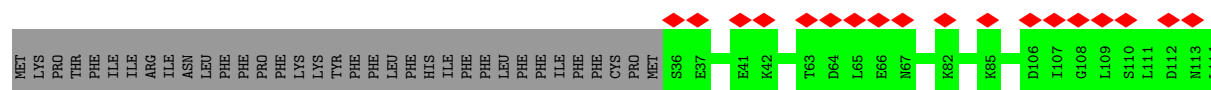
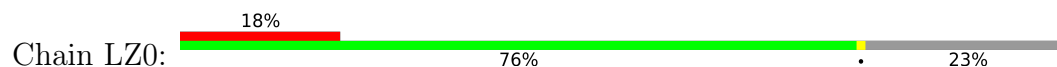
- Molecule 48: 60S ribosomal protein L27

Chain KZ0:  22% 76% 23%

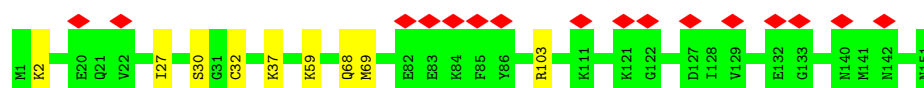




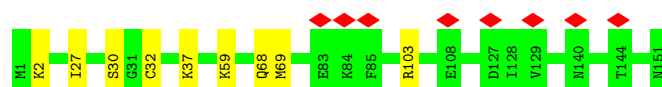
- Molecule 48: 60S ribosomal protein L27



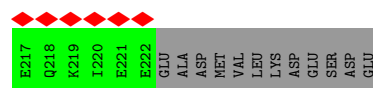
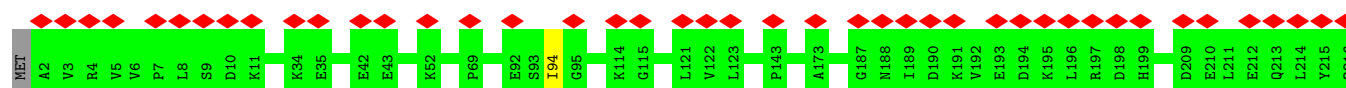
- Molecule 49: DNL-type domain-containing protein



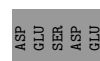
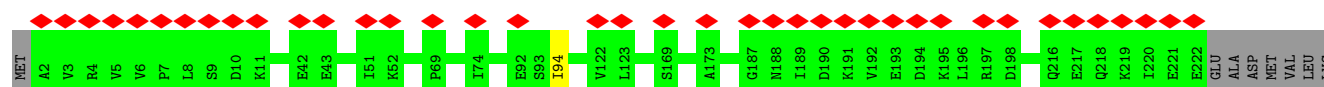
- Molecule 49: DNL-type domain-containing protein



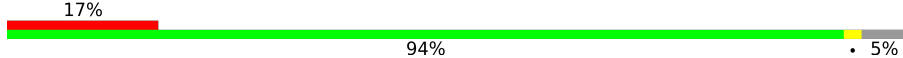
- Molecule 50: 40S ribosomal protein S0



- Molecule 50: 40S ribosomal protein S0

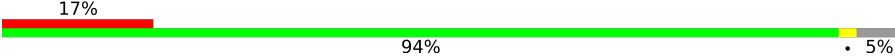


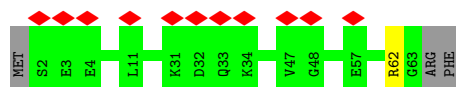
- Molecule 51: 40S ribosomal protein S28

Chain RCC:  17% 94% 5%

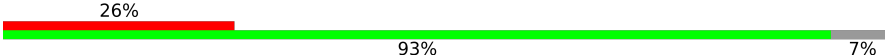


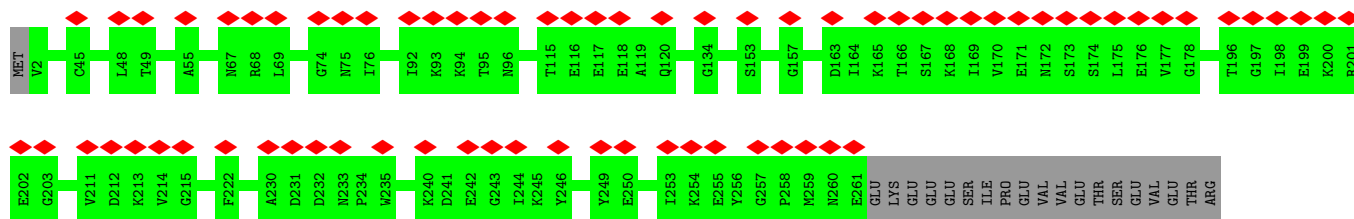
- Molecule 51: 40S ribosomal protein S28

Chain SCC:  17% 94% 5%

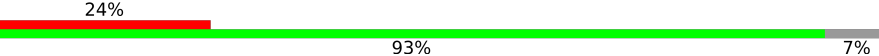


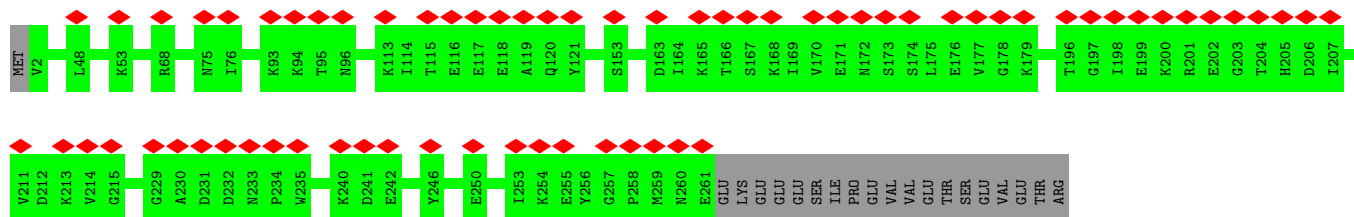
- Molecule 52: 40S ribosomal protein S4

Chain RE0:  26% 93% 7%

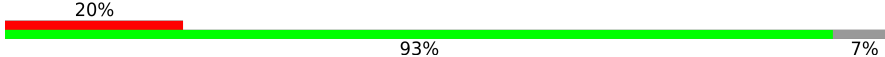


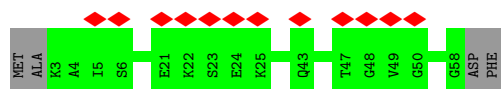
- Molecule 52: 40S ribosomal protein S4

Chain SE0:  24% 93% 7%

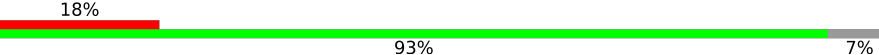


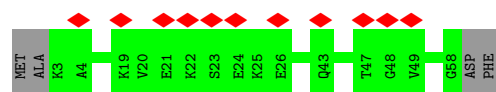
- Molecule 53: 40S ribosomal protein S30

Chain REE:  20% 93% 7%



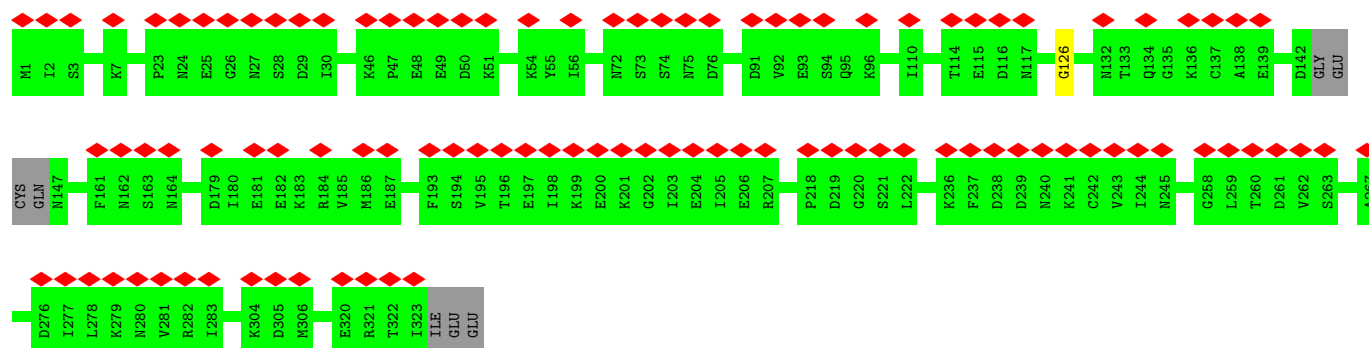
- Molecule 53: 40S ribosomal protein S30

Chain SEE:  18% 93% 7%



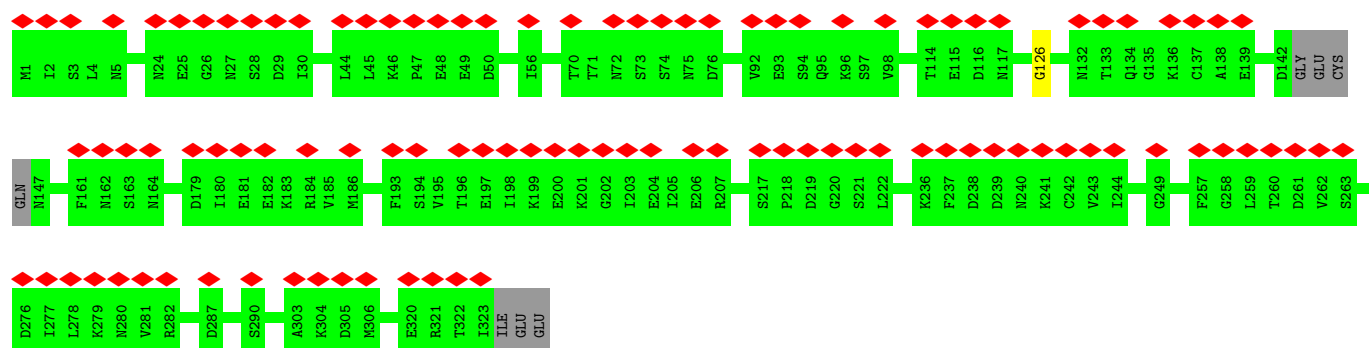
- Molecule 54: Guanine nucleotide binding protein beta subunit

Chain RGG: 32% 98%



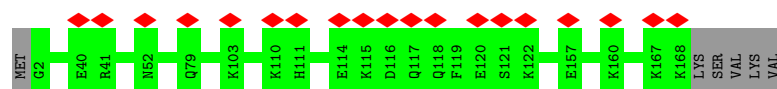
- Molecule 54: Guanine nucleotide binding protein beta subunit

Chain SGG: 32% 98%



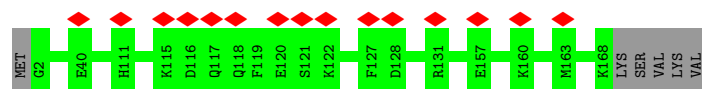
- Molecule 55: 40S ribosomal protein S8

Chain RI0: 11% 97%

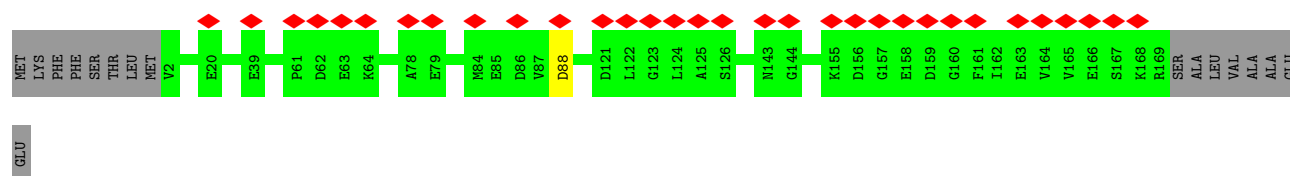


- Molecule 55: 40S ribosomal protein S8

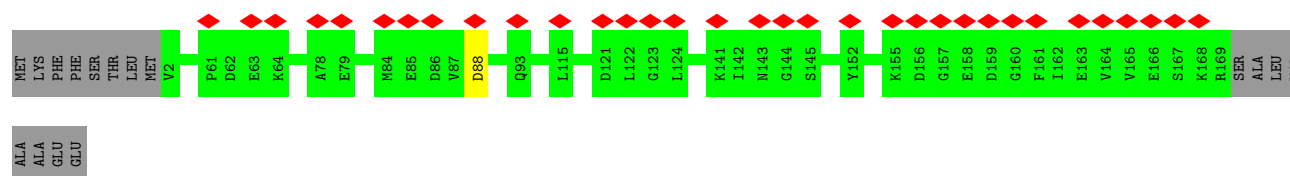
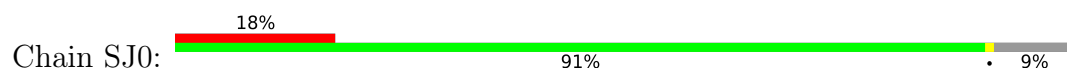
Chain SI0: 9% 97%



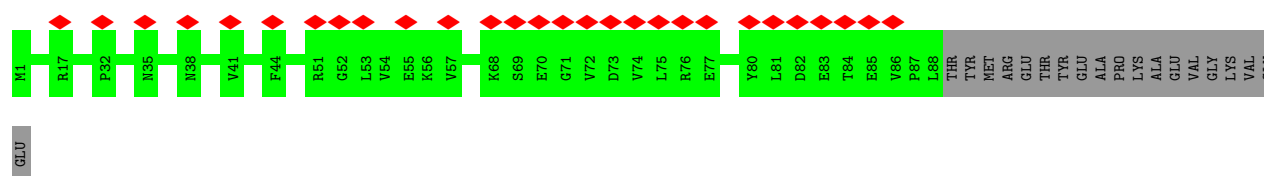
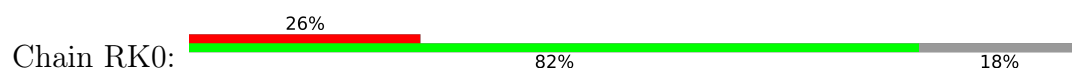
- Molecule 56: 40S ribosomal protein S9



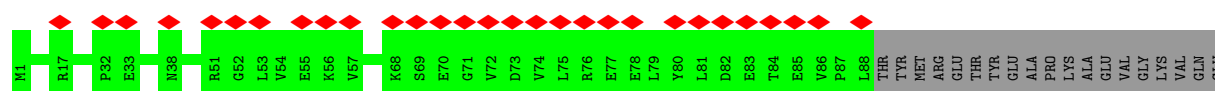
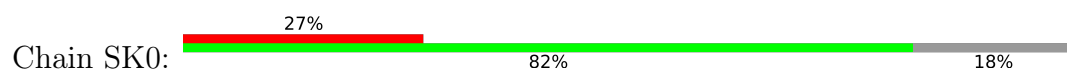
- Molecule 56: 40S ribosomal protein S9



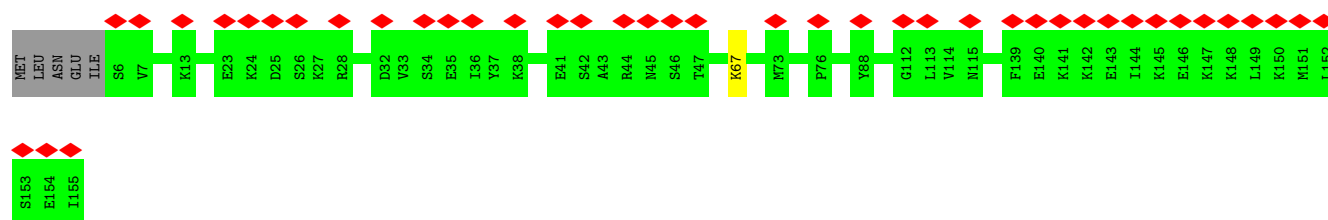
- Molecule 57: 40S ribosomal protein S10



- Molecule 57: 40S ribosomal protein S10

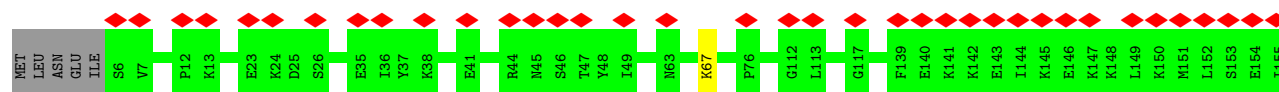


- Molecule 58: 40S ribosomal protein S11

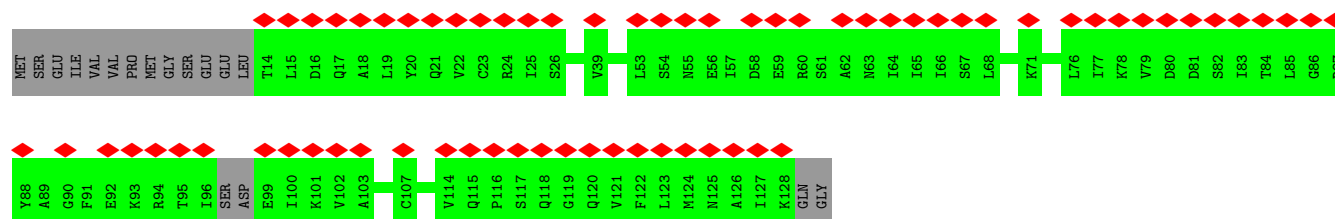
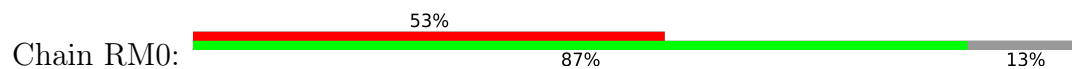


- Molecule 58: 40S ribosomal protein S11

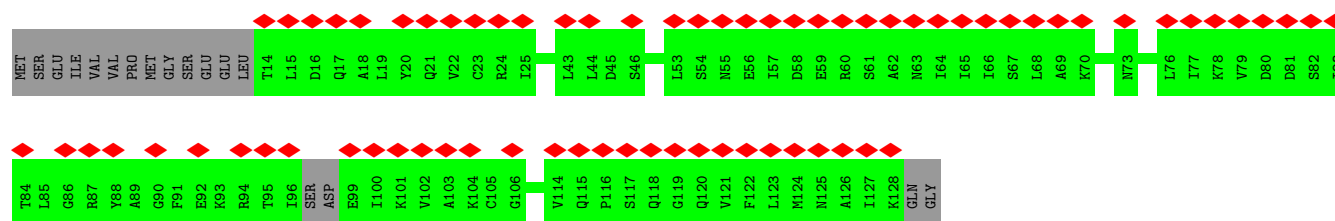
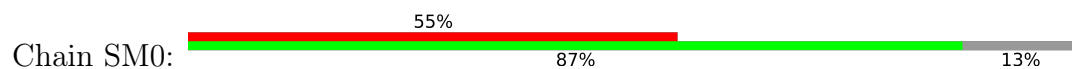




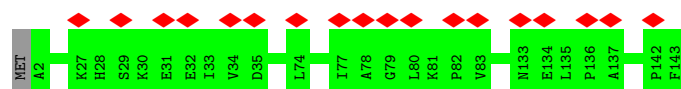
- Molecule 59: 40S ribosomal protein S12



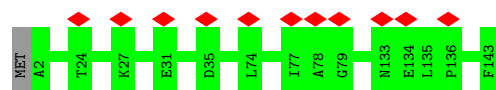
- Molecule 59: 40S ribosomal protein S12



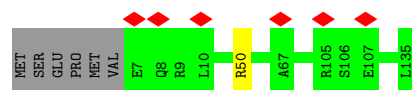
- Molecule 60: 40S ribosomal protein S13



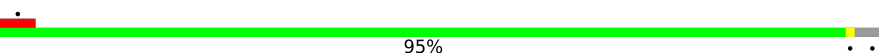
- Molecule 60: 40S ribosomal protein S13

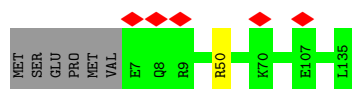


- Molecule 61: 40S ribosomal protein S14



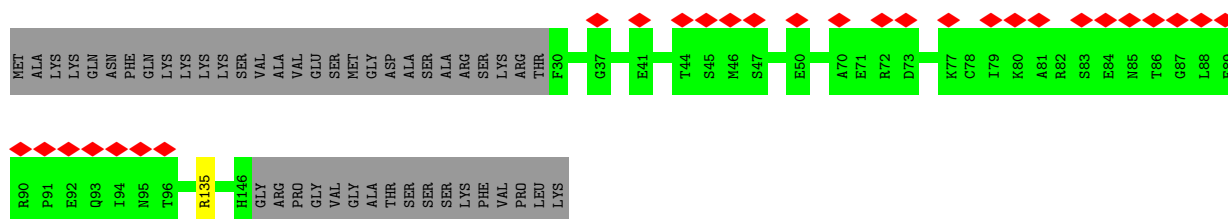
- Molecule 61: 40S ribosomal protein S14

Chain SO0:  95%



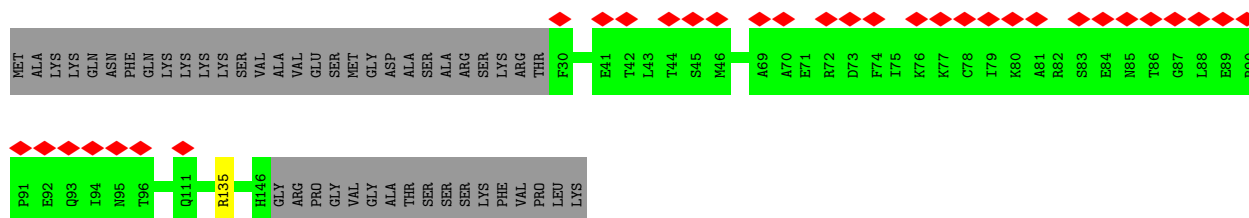
• Molecule 62: Ribosomal protein S19

Chain RP0:  17% 71% 28%

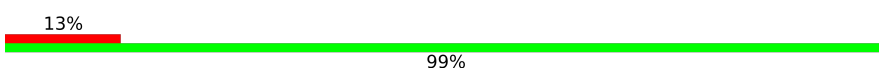


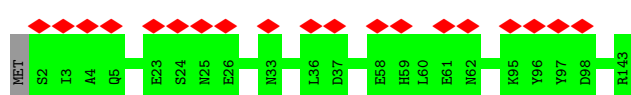
• Molecule 62: Ribosomal protein S19

Chain SP0:  20% 71% 28%

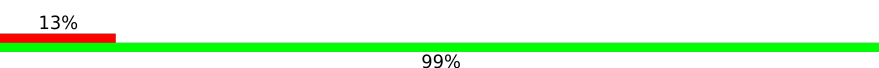


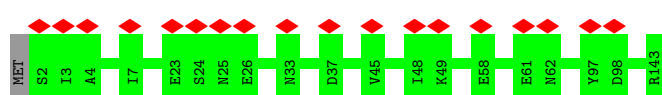
• Molecule 63: 40S ribosomal protein S16

Chain RQ0:  13% 99%

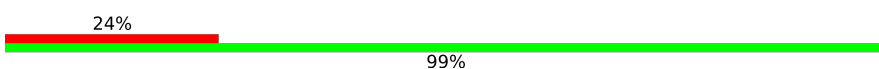


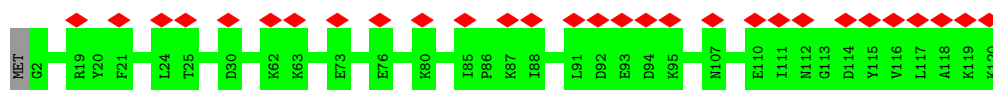
• Molecule 63: 40S ribosomal protein S16

Chain SQ0:  13% 99%

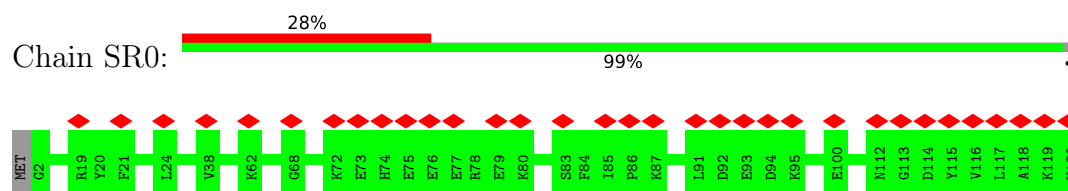


• Molecule 64: 40S ribosomal protein S17

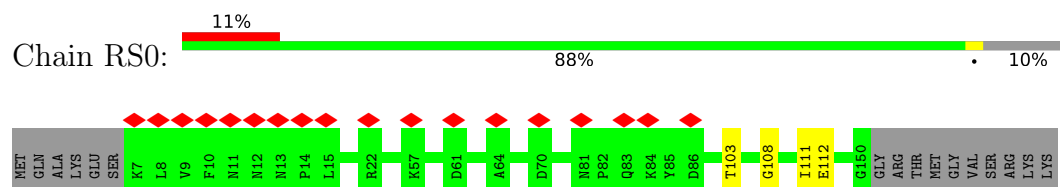
Chain RR0:  24% 99%



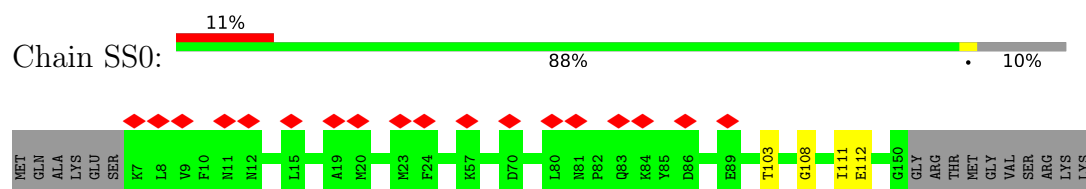
- Molecule 64: 40S ribosomal protein S17



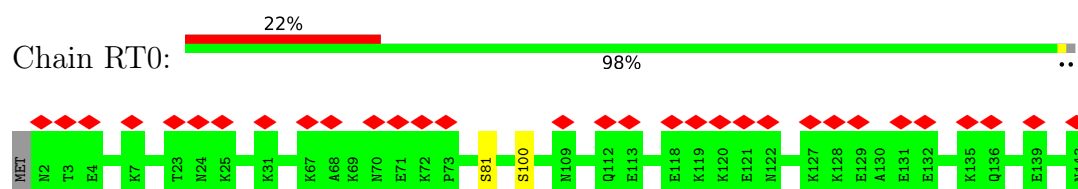
- Molecule 65: 40S ribosomal protein S18



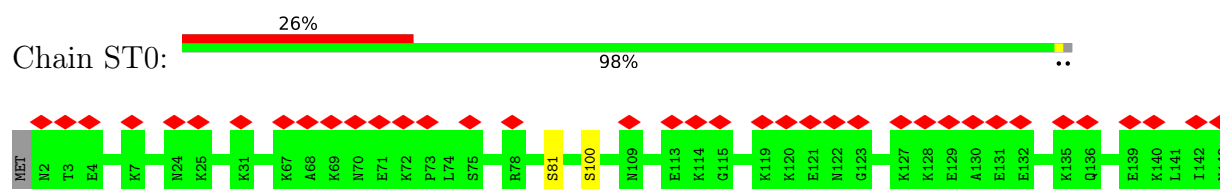
- Molecule 65: 40S ribosomal protein S18



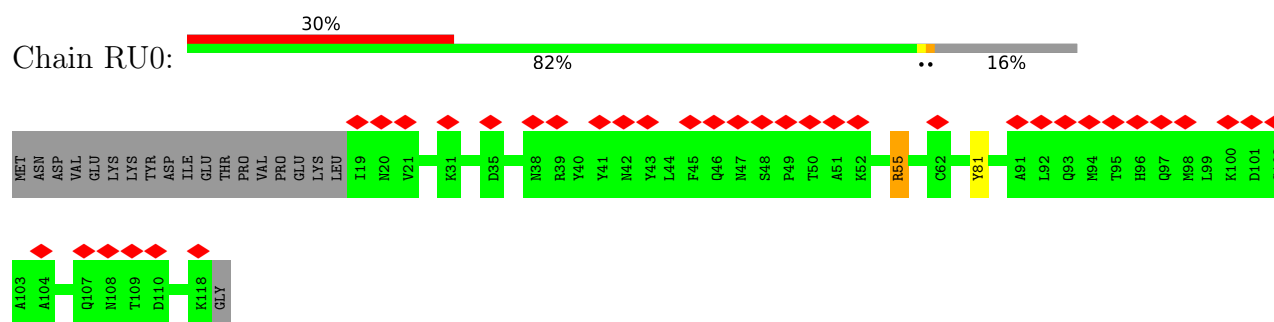
- Molecule 66: 40S Ribosomal protein S19



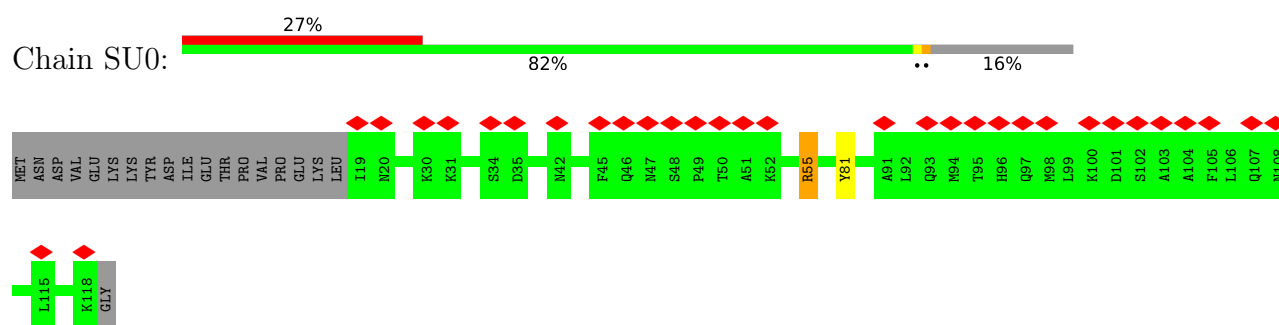
- Molecule 66: 40S Ribosomal protein S19



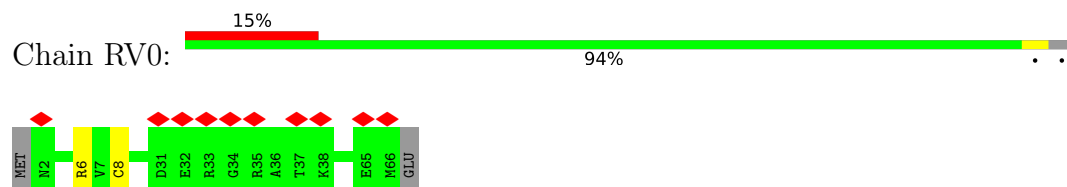
- Molecule 67: 40S ribosomal protein S20



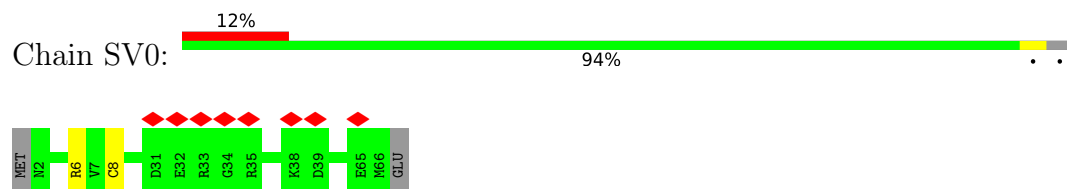
- Molecule 67: 40S ribosomal protein S20



- Molecule 68: Ribosomal protein S21E



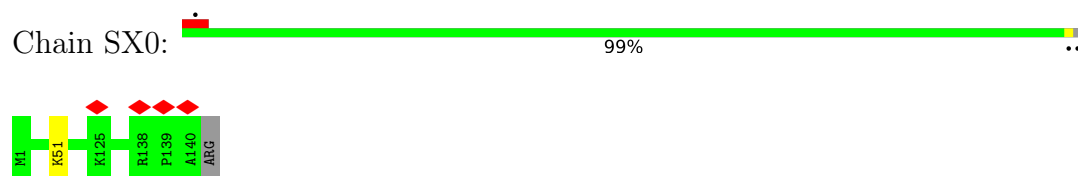
- Molecule 68: Ribosomal protein S21E



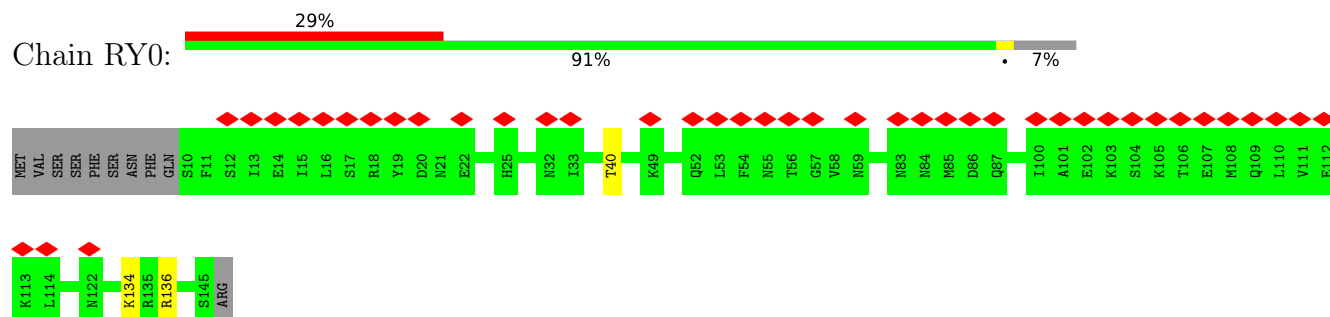
- Molecule 69: 40S ribosomal protein uS12



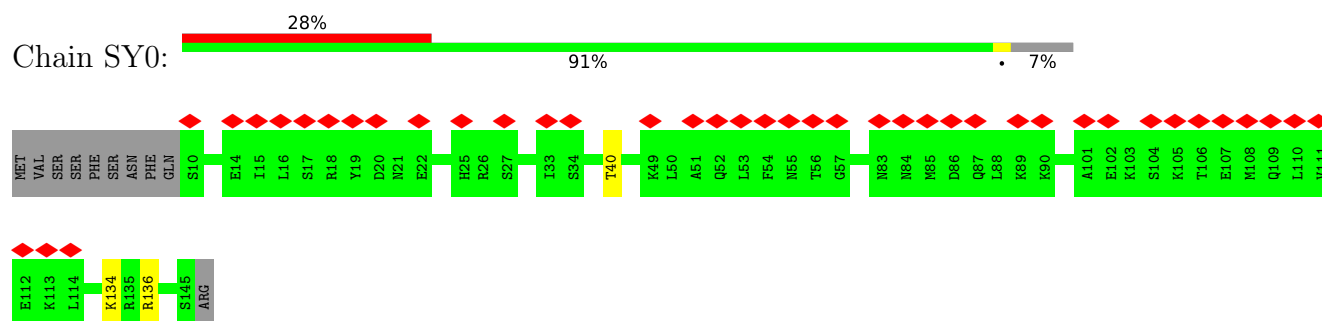
- Molecule 69: 40S ribosomal protein uS12



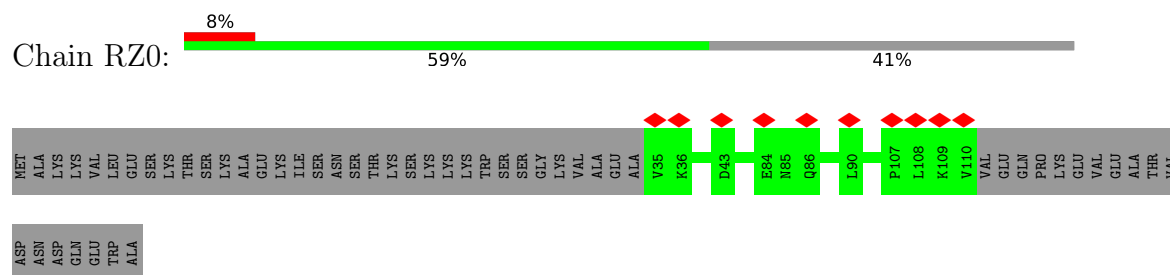
- Molecule 70: 40s ribosomal protein s24



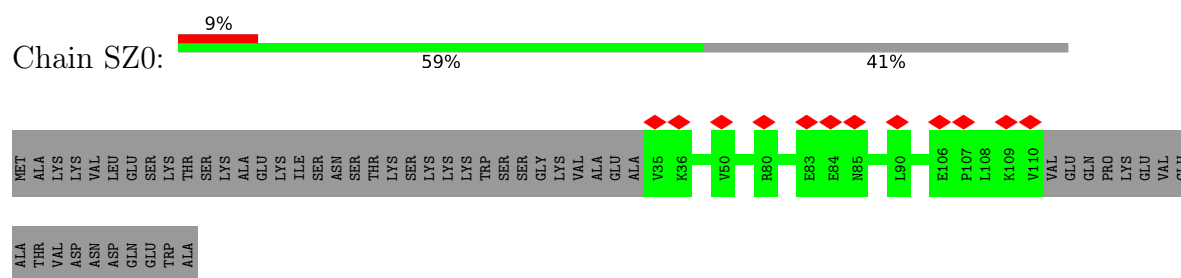
## • Molecule 70: 40s ribosomal protein s24



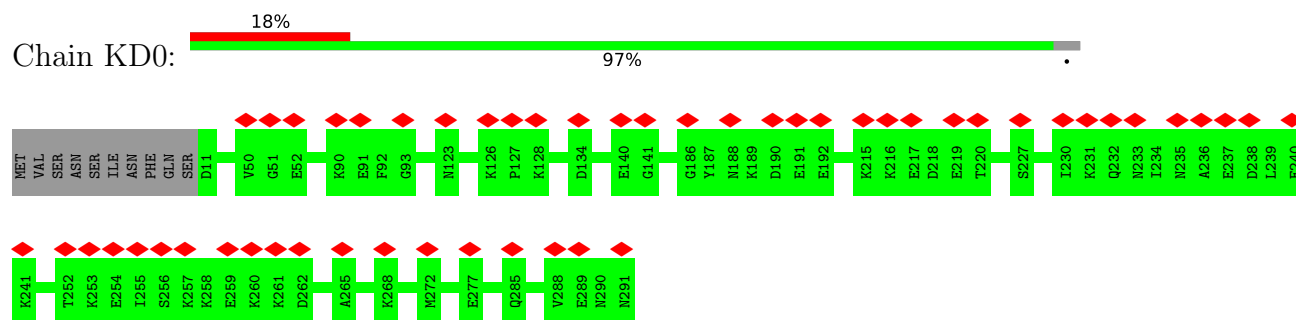
## • Molecule 71: 40S ribosomal protein S25



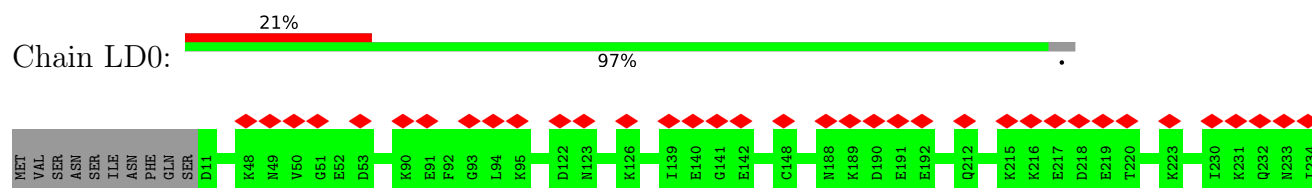
## • Molecule 71: 40S ribosomal protein S25

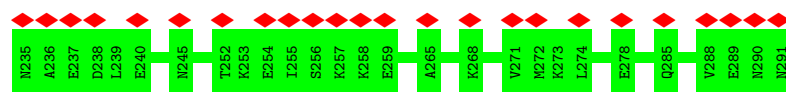


## • Molecule 72: 60S ribosomal protein L5

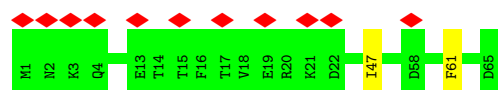


## • Molecule 72: 60S ribosomal protein L5

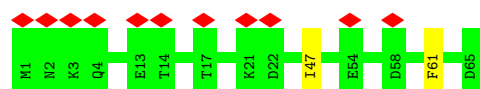




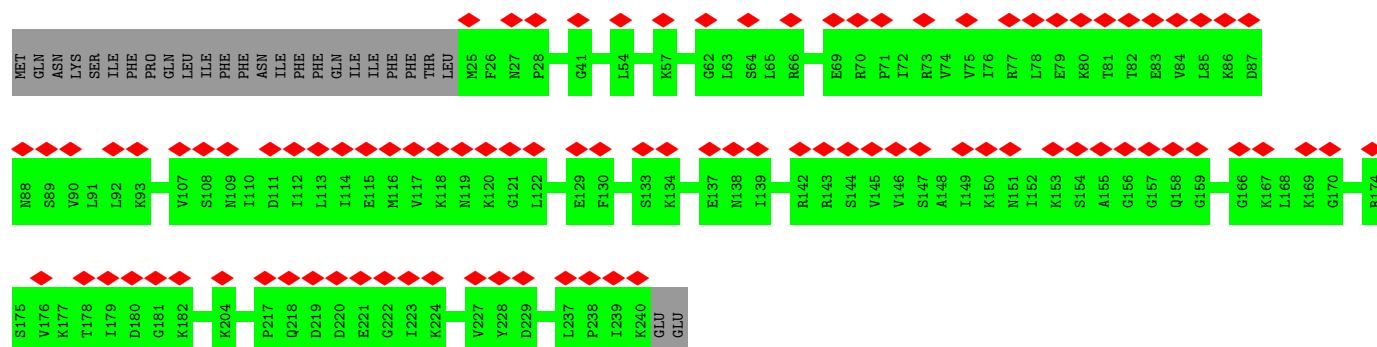
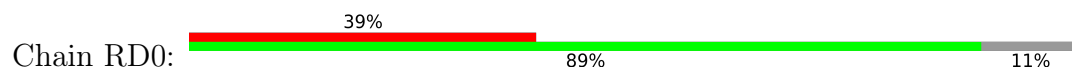
- Molecule 73: 40S ribosomal protein S29



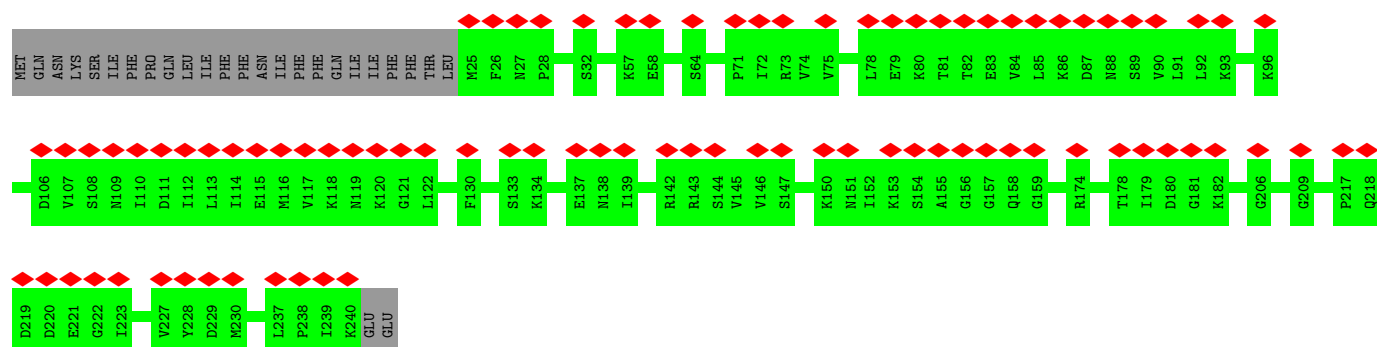
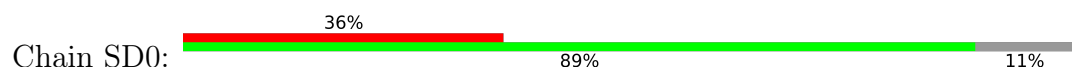
- Molecule 73: 40S ribosomal protein S29



- Molecule 74: 40S ribosomal protein S3



- Molecule 74: 40S ribosomal protein S3



- Molecule 75: 40S ribosomal protein S6

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| M1   | T9   | M10  | F16  | D19  | F20  | K21  | P42  | E43  | W44  | E45  | G46  | L47  | K64  | T65  | G79  | D80  | R92  | I114 | D115 | A116 | K117 | E118 | V119 | A120 | I121 | T125 | D126 | V127 | V128 | S148 | E149 | D150 | A151 | D152 | V153 | T154 | A155 | E156 | L159 | K160 | V161 | I162 | K163 | D164 | A165 | I166 | L167 | F168 |
| V169 | M170 | G171 | G172 | D173 | L177 | V185 | Q186 | T187 | E188 | K191 | E192 | A195 | E196 | K197 | I198 | K199 | E202 | E203 | R204 | K205 | K206 | K207 | S208 | E209 | E211 | R212 | A213 | D214 | F215 | L216 | K217 | K218 | Y219 | P220 | D221 | W222 | Q223 | K224 | K225 | K229 | ALA  |      |      |      |      |      |      |      |

- 
- The diagram illustrates the 16S rRNA gene structure of *E. coli*, showing the positions of various nucleotides and the locations of several antibiotics. The gene is represented as a horizontal bar divided into segments, each labeled with a specific nucleotide position. The segments are color-coded: green for most coding regions, yellow for the 3'-terminal region (R92, R93), and grey for the 5'-terminal region (T228, K229, ALA). Red diamond markers indicate the binding sites for various antibiotics: tetracycline (Tet), streptomycin (Str), chloramphenicol (Chl), erythromycin (Ery), and fusidic acid (Fus). The gene structure includes the 5' UTR (D173, L177), the 16S rRNA coding region (L180 to R92), the 23S rRNA coding region (R93 to T125), the 23S rRNA coding region (T126 to E156), the 23S rRNA coding region (L159 to K160), the 23S rRNA coding region (K163 to E168), and the 3' UTR (G171, G172).

- |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| K119 | E120 | M123 | I124 | K125 | E126 | R133 | K134 | S135 | E136 | F137 | T138 | E139 | E140 | E141 | E151 | L152 | G160 | L161 | Y164 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| MET  | S2   | Q3   | S4   | Q5   | S6   | E7   | M8   | Q9   | E12  | V13  | I14  | K15  | V17  | C18  | G19  | S20  | V21  | T22  | K23  | D24 | Q27 | S28 | K31 | K36 | L37 | I38 | S39 | D40 | S41 | D42 | G43 | S44 | N45 | L51 | L55 | A58 | E65 | M68 | K69 | L70 | Q71 | K72 | Q73 | F74 | S75 | E76 | F81 |

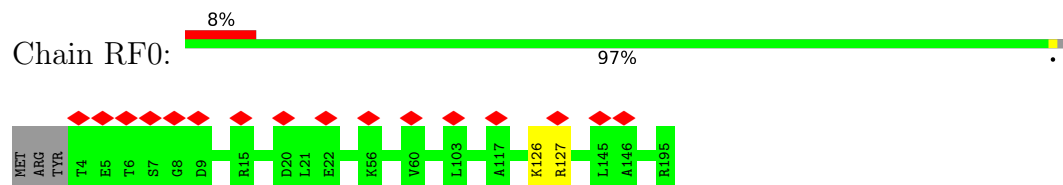
- [illegible]

- 
- | Cluster | Number of Genes |
|---------|-----------------|
| M1      | 1               |
| L8      | 8               |
| A18     | 18              |
| R33     | 33              |
| L34     | 34              |
| T46     | 46              |
| D47     | 47              |
| E56     | 56              |
| R66     | 66              |
| E85     | 85              |
| R95     | 95              |
| G96     | 96              |
| K106    | 106             |
| Q116    | 116             |
| H117    | 117             |
| N118    | 118             |
| Y128    | 128             |

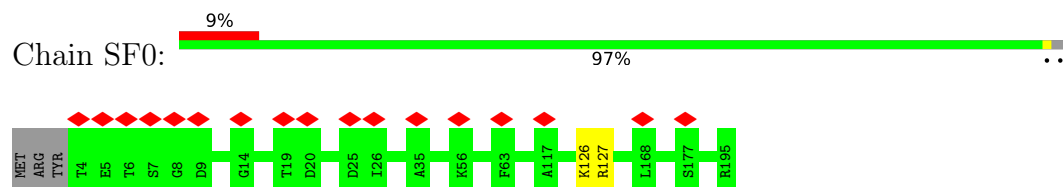
- Molecule 77: 40S ribosomal protein S15A



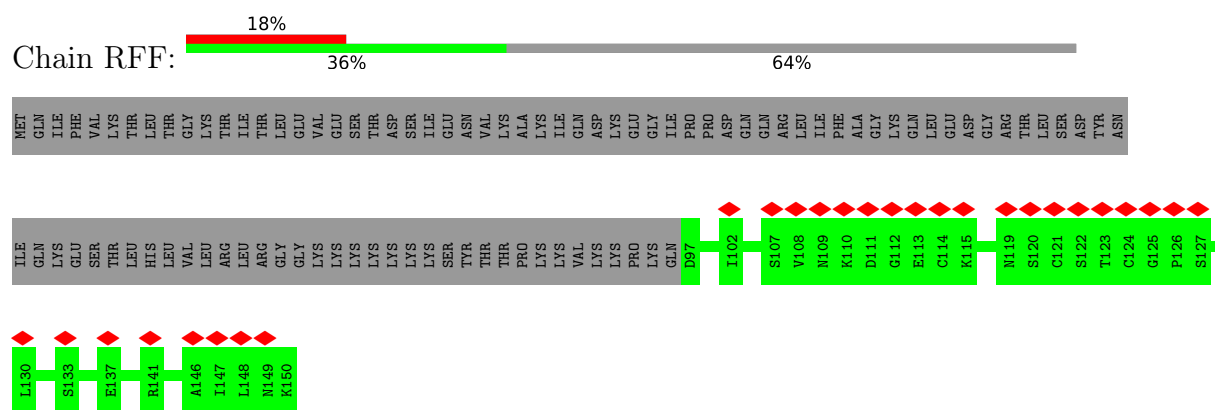
- Molecule 78: 40S ribosomal protein S5



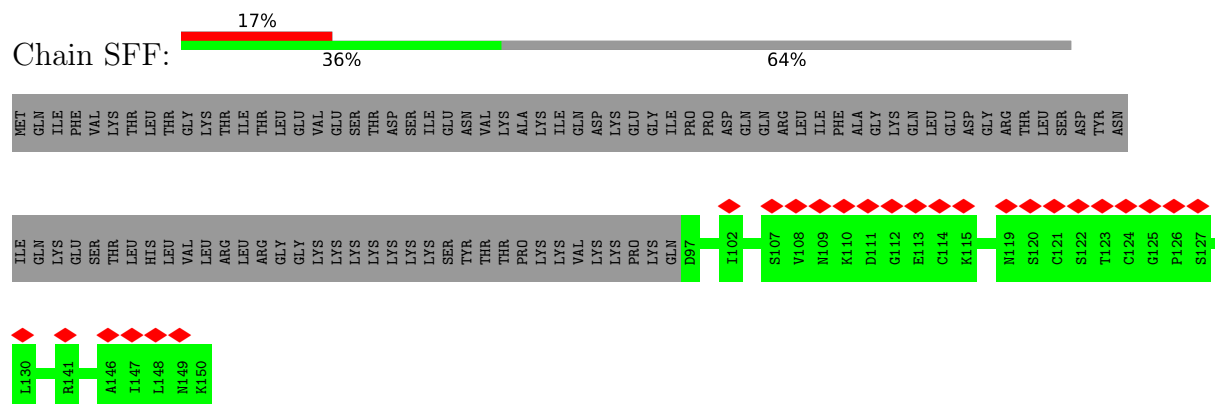
- Molecule 78: 40S ribosomal protein S5



- Molecule 79: Ubiquitin/40s ribosomal protein S27a fusion



- Molecule 79: Ubiquitin/40s ribosomal protein S27a fusion



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SUBTOMOGRAM AVERAGING                   | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of subtomograms used          | 3109                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 120                                     | Depositor |
| Minimum defocus (nm)                 | 3000                                    | Depositor |
| Maximum defocus (nm)                 | 5000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 2.637                                   | Depositor |
| Minimum map value                    | -1.019                                  | Depositor |
| Average map value                    | 0.017                                   | Depositor |
| Map value standard deviation         | 0.197                                   | Depositor |
| Recommended contour level            | 0.25                                    | Depositor |
| Map size (Å)                         | 588.0, 588.0, 588.0                     | wwPDB     |
| Map dimensions                       | 168, 168, 168                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 3.5, 3.5, 3.5                           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | K50   | 0.47         | 7/62688 (0.0%) | 0.92        | 143/97791 (0.1%) |
| 1   | L50   | 0.47         | 7/62688 (0.0%) | 0.92        | 143/97791 (0.1%) |
| 2   | R60   | 0.42         | 0/32724        | 1.01        | 96/51066 (0.2%)  |
| 2   | S60   | 0.42         | 0/32724        | 1.01        | 96/51066 (0.2%)  |
| 3   | D     | 0.24         | 0/1234         | 0.61        | 0/1662           |
| 3   | E     | 0.24         | 0/1234         | 0.61        | 0/1662           |
| 4   | KGG   | 0.29         | 0/825          | 0.61        | 0/1090           |
| 4   | LGG   | 0.29         | 0/825          | 0.61        | 0/1090           |
| 5   | RB0   | 0.21         | 0/1623         | 0.47        | 0/2169           |
| 5   | SB0   | 0.21         | 0/1623         | 0.47        | 0/2169           |
| 6   | RC0   | 0.21         | 0/1755         | 0.52        | 0/2364           |
| 6   | SC0   | 0.21         | 0/1755         | 0.52        | 0/2364           |
| 7   | K70   | 0.41         | 0/2843         | 0.86        | 2/4429 (0.0%)    |
| 7   | L70   | 0.41         | 0/2843         | 0.86        | 2/4429 (0.0%)    |
| 8   | A     | 0.32         | 0/6717         | 0.67        | 2/9049 (0.0%)    |
| 8   | B     | 0.32         | 0/6717         | 0.67        | 2/9049 (0.0%)    |
| 9   | K     | 0.19         | 0/1747         | 0.47        | 0/2333           |
| 9   | L     | 0.19         | 0/1747         | 0.47        | 0/2333           |
| 10  | M     | 0.23         | 0/2138         | 0.50        | 0/2865           |
| 10  | N     | 0.23         | 0/2138         | 0.50        | 0/2865           |
| 11  | KMM   | 0.55         | 0/431          | 0.78        | 0/568            |
| 11  | LMM   | 0.55         | 0/431          | 0.78        | 0/568            |
| 12  | RBB   | 0.18         | 0/634          | 0.45        | 0/844            |
| 12  | SBB   | 0.18         | 0/634          | 0.45        | 0/844            |
| 13  | RAA   | 0.20         | 0/839          | 0.54        | 0/1120           |
| 13  | SAA   | 0.20         | 0/839          | 0.54        | 0/1120           |
| 14  | KOO   | 0.22         | 0/811          | 0.57        | 0/1071           |
| 14  | LOO   | 0.22         | 0/811          | 0.57        | 0/1071           |
| 15  | KPP   | 0.24         | 0/693          | 0.65        | 0/918            |
| 15  | LPP   | 0.24         | 0/693          | 0.65        | 0/918            |
| 16  | KJJ   | 0.23         | 0/710          | 0.53        | 0/932            |
| 16  | LJJ   | 0.23         | 0/710          | 0.53        | 0/932            |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 17  | LA0   | 0.31         | 1/1926 (0.1%) | 0.51        | 1/2590 (0.0%) |
| 17  | LA02  | 0.31         | 1/1926 (0.1%) | 0.51        | 1/2590 (0.0%) |
| 18  | KAA   | 0.27         | 0/1191        | 0.66        | 1/1586 (0.1%) |
| 18  | LAA   | 0.27         | 0/1191        | 0.66        | 1/1586 (0.1%) |
| 19  | KB0   | 0.25         | 0/3092        | 0.54        | 1/4144 (0.0%) |
| 19  | LB0   | 0.25         | 0/3092        | 0.54        | 1/4144 (0.0%) |
| 20  | KC0   | 0.22         | 0/2646        | 0.54        | 0/3555        |
| 20  | LC0   | 0.22         | 0/2646        | 0.54        | 0/3555        |
| 21  | KCC   | 0.21         | 0/794         | 0.45        | 0/1067        |
| 21  | LCC   | 0.21         | 0/794         | 0.45        | 0/1067        |
| 22  | KDD   | 0.21         | 0/913         | 0.49        | 0/1223        |
| 22  | LDD   | 0.21         | 0/913         | 0.49        | 0/1223        |
| 23  | KE0   | 0.21         | 0/1394        | 0.52        | 1/1875 (0.1%) |
| 23  | LE0   | 0.21         | 0/1394        | 0.52        | 1/1875 (0.1%) |
| 24  | KEE   | 0.36         | 0/1108        | 0.72        | 2/1477 (0.1%) |
| 24  | LEE   | 0.36         | 0/1108        | 0.72        | 2/1477 (0.1%) |
| 25  | KF0   | 0.23         | 0/1963        | 0.51        | 0/2618        |
| 25  | LF0   | 0.23         | 0/1963        | 0.51        | 0/2618        |
| 26  | KFF   | 0.23         | 0/906         | 0.53        | 0/1207        |
| 26  | LFF   | 0.23         | 0/906         | 0.53        | 0/1207        |
| 27  | KG0   | 0.23         | 0/1612        | 0.52        | 0/2163        |
| 27  | LG0   | 0.23         | 0/1612        | 0.52        | 0/2163        |
| 28  | KH0   | 0.26         | 0/1503        | 0.52        | 0/2018        |
| 28  | LH0   | 0.26         | 0/1503        | 0.52        | 0/2018        |
| 29  | KHH   | 0.34         | 0/1000        | 0.69        | 1/1324 (0.1%) |
| 29  | LHH   | 0.34         | 0/1000        | 0.69        | 1/1324 (0.1%) |
| 30  | KI0   | 0.22         | 0/1781        | 0.53        | 0/2382        |
| 30  | LI0   | 0.22         | 0/1781        | 0.53        | 0/2382        |
| 31  | KII   | 0.20         | 0/790         | 0.50        | 0/1041        |
| 31  | LII   | 0.20         | 0/790         | 0.50        | 0/1041        |
| 32  | KJ0   | 0.21         | 0/1350        | 0.56        | 0/1797        |
| 32  | LJ0   | 0.21         | 0/1350        | 0.56        | 0/1797        |
| 33  | KL0   | 0.45         | 2/1374 (0.1%) | 0.77        | 2/1827 (0.1%) |
| 33  | LL0   | 0.45         | 2/1374 (0.1%) | 0.77        | 2/1827 (0.1%) |
| 34  | KLL   | 0.24         | 0/435         | 0.55        | 0/576         |
| 34  | LLL   | 0.24         | 0/435         | 0.55        | 0/576         |
| 35  | KM0   | 0.20         | 0/935         | 0.50        | 0/1251        |
| 35  | LM0   | 0.20         | 0/935         | 0.50        | 0/1251        |
| 36  | KN0   | 0.26         | 0/1722        | 0.65        | 0/2297        |
| 36  | LN0   | 0.26         | 0/1722        | 0.65        | 0/2297        |
| 37  | KO0   | 0.23         | 0/1626        | 0.53        | 0/2168        |
| 37  | LO0   | 0.23         | 0/1626        | 0.53        | 0/2168        |
| 38  | KP0   | 0.22         | 0/1262        | 0.51        | 0/1689        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 38  | LP0   | 0.22         | 0/1262  | 0.51        | 0/1689        |
| 39  | KQ0   | 0.29         | 0/1512  | 0.61        | 1/2014 (0.0%) |
| 39  | LQ0   | 0.29         | 0/1512  | 0.61        | 1/2014 (0.0%) |
| 40  | KR0   | 0.24         | 0/1352  | 0.55        | 0/1790        |
| 40  | LR0   | 0.24         | 0/1352  | 0.55        | 0/1790        |
| 41  | KS0   | 0.25         | 0/1422  | 0.53        | 0/1898        |
| 41  | LS0   | 0.25         | 0/1422  | 0.53        | 0/1898        |
| 42  | KT0   | 0.22         | 0/1294  | 0.52        | 0/1736        |
| 42  | LT0   | 0.22         | 0/1294  | 0.52        | 0/1736        |
| 43  | KU0   | 0.20         | 0/826   | 0.45        | 0/1104        |
| 43  | LU0   | 0.20         | 0/826   | 0.45        | 0/1104        |
| 44  | KV0   | 0.22         | 0/1068  | 0.56        | 0/1429        |
| 44  | LV0   | 0.22         | 0/1068  | 0.56        | 0/1429        |
| 45  | KW0   | 0.18         | 0/849   | 0.45        | 0/1129        |
| 45  | LW0   | 0.18         | 0/849   | 0.45        | 0/1129        |
| 46  | KX0   | 0.20         | 0/883   | 0.45        | 0/1175        |
| 46  | LX0   | 0.20         | 0/883   | 0.45        | 0/1175        |
| 47  | KY0   | 0.23         | 0/1058  | 0.53        | 0/1399        |
| 47  | LY0   | 0.23         | 0/1058  | 0.53        | 0/1399        |
| 48  | KZ0   | 0.36         | 0/976   | 0.59        | 0/1302        |
| 48  | LZ0   | 0.36         | 0/976   | 0.59        | 0/1302        |
| 49  | MD1   | 0.52         | 0/1249  | 0.97        | 4/1677 (0.2%) |
| 49  | ND1   | 0.52         | 0/1249  | 0.97        | 4/1677 (0.2%) |
| 50  | RA0   | 0.21         | 0/1751  | 0.53        | 1/2358 (0.0%) |
| 50  | SA0   | 0.21         | 0/1751  | 0.53        | 1/2358 (0.0%) |
| 51  | RCC   | 0.19         | 0/480   | 0.48        | 0/644         |
| 51  | SCC   | 0.19         | 0/480   | 0.48        | 0/644         |
| 52  | RE0   | 0.20         | 0/2080  | 0.52        | 0/2804        |
| 52  | SE0   | 0.20         | 0/2080  | 0.52        | 0/2804        |
| 53  | REE   | 0.20         | 0/453   | 0.51        | 0/596         |
| 53  | SEE   | 0.20         | 0/453   | 0.51        | 0/596         |
| 54  | RGG   | 0.19         | 0/2517  | 0.51        | 0/3397        |
| 54  | SGG   | 0.19         | 0/2517  | 0.51        | 0/3397        |
| 55  | RI0   | 0.23         | 0/1369  | 0.54        | 0/1825        |
| 55  | SI0   | 0.23         | 0/1369  | 0.54        | 0/1825        |
| 56  | RJ0   | 0.22         | 0/1403  | 0.56        | 0/1880        |
| 56  | SJ0   | 0.22         | 0/1403  | 0.56        | 0/1880        |
| 57  | RK0   | 0.25         | 0/750   | 0.59        | 0/1009        |
| 57  | SK0   | 0.25         | 0/750   | 0.59        | 0/1009        |
| 58  | RL0   | 0.19         | 0/1252  | 0.45        | 0/1672        |
| 58  | SL0   | 0.19         | 0/1252  | 0.45        | 0/1672        |
| 59  | RM0   | 0.16         | 0/881   | 0.40        | 0/1182        |
| 59  | SM0   | 0.16         | 0/881   | 0.40        | 0/1182        |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 60  | RN0   | 0.25         | 0/1154           | 0.47        | 0/1557            |
| 60  | SN0   | 0.25         | 0/1154           | 0.47        | 0/1557            |
| 61  | RO0   | 0.23         | 0/993            | 0.58        | 0/1326            |
| 61  | SO0   | 0.23         | 0/993            | 0.58        | 0/1326            |
| 62  | RP0   | 0.25         | 0/964            | 0.61        | 0/1289            |
| 62  | SP0   | 0.25         | 0/964            | 0.61        | 0/1289            |
| 63  | RQ0   | 0.23         | 0/1163           | 0.54        | 0/1556            |
| 63  | SQ0   | 0.23         | 0/1163           | 0.54        | 0/1556            |
| 64  | RR0   | 0.24         | 0/985            | 0.60        | 0/1315            |
| 64  | SR0   | 0.24         | 0/985            | 0.60        | 0/1315            |
| 65  | RS0   | 0.23         | 0/1165           | 0.64        | 0/1566            |
| 65  | SS0   | 0.23         | 0/1165           | 0.64        | 0/1566            |
| 66  | RT0   | 0.21         | 0/1181           | 0.56        | 0/1585            |
| 66  | ST0   | 0.21         | 0/1181           | 0.56        | 0/1585            |
| 67  | RU0   | 0.24         | 0/824            | 0.58        | 0/1110            |
| 67  | SU0   | 0.24         | 0/824            | 0.58        | 0/1110            |
| 68  | RV0   | 0.25         | 0/525            | 0.74        | 0/700             |
| 68  | SV0   | 0.25         | 0/525            | 0.74        | 0/700             |
| 69  | RX0   | 0.23         | 0/1113           | 0.62        | 0/1486            |
| 69  | SX0   | 0.23         | 0/1113           | 0.62        | 0/1486            |
| 70  | RY0   | 0.19         | 0/1131           | 0.58        | 0/1503            |
| 70  | SY0   | 0.19         | 0/1131           | 0.58        | 0/1503            |
| 71  | RZ0   | 0.22         | 0/640            | 0.58        | 0/855             |
| 71  | SZ0   | 0.22         | 0/640            | 0.58        | 0/855             |
| 72  | KD0   | 0.18         | 0/2328           | 0.46        | 0/3098            |
| 72  | LD0   | 0.18         | 0/2328           | 0.46        | 0/3098            |
| 73  | RDD   | 0.28         | 0/559            | 0.71        | 0/742             |
| 73  | SDD   | 0.28         | 0/559            | 0.71        | 0/742             |
| 74  | RD0   | 0.18         | 0/1721           | 0.46        | 0/2304            |
| 74  | SD0   | 0.18         | 0/1721           | 0.46        | 0/2304            |
| 75  | RG0   | 0.20         | 0/1863           | 0.53        | 0/2483            |
| 75  | SG0   | 0.20         | 0/1863           | 0.53        | 0/2483            |
| 76  | RH0   | 0.19         | 0/1356           | 0.49        | 0/1820            |
| 76  | SH0   | 0.19         | 0/1356           | 0.49        | 0/1820            |
| 77  | RW0   | 0.23         | 0/1037           | 0.60        | 0/1389            |
| 77  | SW0   | 0.23         | 0/1037           | 0.60        | 0/1389            |
| 78  | RF0   | 0.25         | 0/1527           | 0.61        | 2/2045 (0.1%)     |
| 78  | SF0   | 0.25         | 0/1527           | 0.61        | 2/2045 (0.1%)     |
| 79  | RFF   | 0.58         | 0/418            | 0.98        | 0/560             |
| 79  | SFF   | 0.58         | 0/418            | 0.98        | 0/560             |
| All | All   | 0.36         | 20/395614 (0.0%) | 0.79        | 520/572910 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | K50   | 0                   | 13                  |
| 1   | L50   | 0                   | 13                  |
| 8   | A     | 0                   | 5                   |
| 8   | B     | 0                   | 5                   |
| 29  | KHH   | 0                   | 1                   |
| 29  | LHH   | 0                   | 1                   |
| 32  | KJ0   | 0                   | 1                   |
| 32  | LJ0   | 0                   | 1                   |
| 48  | KZ0   | 0                   | 1                   |
| 48  | LZ0   | 0                   | 1                   |
| 54  | RGG   | 0                   | 1                   |
| 54  | SGG   | 0                   | 1                   |
| 56  | RJ0   | 0                   | 1                   |
| 56  | SJ0   | 0                   | 1                   |
| 61  | RO0   | 0                   | 1                   |
| 61  | SO0   | 0                   | 1                   |
| 65  | RS0   | 0                   | 4                   |
| 65  | SS0   | 0                   | 4                   |
| 66  | RT0   | 0                   | 2                   |
| 66  | ST0   | 0                   | 2                   |
| 67  | RU0   | 0                   | 2                   |
| 67  | SU0   | 0                   | 2                   |
| 68  | RV0   | 0                   | 2                   |
| 68  | SV0   | 0                   | 2                   |
| 70  | RY0   | 0                   | 1                   |
| 70  | SY0   | 0                   | 1                   |
| 73  | RDD   | 0                   | 2                   |
| 73  | SDD   | 0                   | 2                   |
| 75  | RG0   | 0                   | 1                   |
| 75  | SG0   | 0                   | 1                   |
| All | All   | 0                   | 76                  |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33  | KL0   | 1   | MET  | CG-SD   | -7.84 | 1.61        | 1.80     |
| 33  | LL0   | 1   | MET  | CG-SD   | -7.84 | 1.61        | 1.80     |
| 17  | LA0   | 180 | TYR  | CD1-CE1 | 7.22  | 1.60        | 1.38     |
| 17  | LA02  | 180 | TYR  | CD1-CE1 | 7.22  | 1.60        | 1.38     |
| 1   | K50   | 311 | C    | C3'-O3' | 6.12  | 1.50        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | L50   | 311 | C    | C3'-O3' | 6.12  | 1.50        | 1.42     |
| 1   | K50   | 179 | U    | C5'-C4' | 5.69  | 1.55        | 1.51     |
| 1   | L50   | 179 | U    | C5'-C4' | 5.69  | 1.55        | 1.51     |
| 33  | KL0   | 1   | MET  | SD-CE   | -5.57 | 1.65        | 1.79     |
| 33  | LL0   | 1   | MET  | SD-CE   | -5.57 | 1.65        | 1.79     |
| 1   | L50   | 178 | G    | C4'-O4' | -5.53 | 1.40        | 1.45     |
| 1   | K50   | 178 | G    | C4'-O4' | -5.53 | 1.40        | 1.45     |
| 1   | K50   | 367 | A    | C5-C4   | -5.50 | 1.34        | 1.38     |
| 1   | L50   | 367 | A    | C5-C4   | -5.50 | 1.34        | 1.38     |
| 1   | K50   | 310 | A    | C5-C4   | -5.11 | 1.35        | 1.38     |
| 1   | L50   | 310 | A    | C5-C4   | -5.11 | 1.35        | 1.38     |
| 1   | L50   | 483 | A    | C5-C4   | -5.07 | 1.35        | 1.38     |
| 1   | K50   | 483 | A    | C5-C4   | -5.07 | 1.35        | 1.38     |
| 1   | K50   | 311 | C    | C5'-C4' | 5.03  | 1.54        | 1.51     |
| 1   | L50   | 311 | C    | C5'-C4' | 5.03  | 1.54        | 1.51     |

All (520) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 2   | R60   | 355  | C    | N1-C2-O2   | 11.55  | 125.83      | 118.90   |
| 2   | S60   | 355  | C    | N1-C2-O2   | 11.55  | 125.83      | 118.90   |
| 1   | K50   | 366  | G    | O4'-C1'-N9 | 11.54  | 116.58      | 108.50   |
| 1   | L50   | 366  | G    | O4'-C1'-N9 | 11.54  | 116.58      | 108.50   |
| 1   | K50   | 202  | G    | O4'-C1'-N9 | 11.34  | 116.44      | 108.50   |
| 1   | L50   | 202  | G    | O4'-C1'-N9 | 11.34  | 116.44      | 108.50   |
| 1   | K50   | 485  | A    | N1-C6-N6   | -10.86 | 112.08      | 118.60   |
| 1   | L50   | 485  | A    | N1-C6-N6   | -10.86 | 112.08      | 118.60   |
| 1   | K50   | 1928 | C    | P-O3'-C3'  | 10.85  | 132.71      | 119.70   |
| 1   | L50   | 1928 | C    | P-O3'-C3'  | 10.85  | 132.71      | 119.70   |
| 1   | K50   | 236  | A    | N1-C6-N6   | -9.33  | 113.00      | 118.60   |
| 1   | L50   | 236  | A    | N1-C6-N6   | -9.33  | 113.00      | 118.60   |
| 2   | R60   | 980  | G    | O4'-C1'-N9 | 9.22   | 115.58      | 108.20   |
| 2   | S60   | 980  | G    | O4'-C1'-N9 | 9.22   | 115.58      | 108.20   |
| 2   | R60   | 1341 | A    | P-O3'-C3'  | -9.18  | 108.68      | 119.70   |
| 2   | S60   | 1341 | A    | P-O3'-C3'  | -9.18  | 108.68      | 119.70   |
| 1   | K50   | 201  | A    | N1-C6-N6   | -8.97  | 113.22      | 118.60   |
| 1   | L50   | 201  | A    | N1-C6-N6   | -8.96  | 113.22      | 118.60   |
| 1   | K50   | 311  | C    | N1-C1'-C2' | 8.87   | 121.75      | 112.00   |
| 1   | L50   | 311  | C    | N1-C1'-C2' | 8.87   | 121.75      | 112.00   |
| 1   | K50   | 366  | G    | N9-C1'-C2' | -8.84  | 102.28      | 112.00   |
| 1   | L50   | 366  | G    | N9-C1'-C2' | -8.84  | 102.28      | 112.00   |
| 1   | L50   | 483  | A    | C5-C6-N1   | 8.72   | 122.06      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | K50   | 483  | A    | C5-C6-N1    | 8.71  | 122.06      | 117.70   |
| 1   | K50   | 310  | A    | C5-C6-N1    | 8.66  | 122.03      | 117.70   |
| 1   | L50   | 310  | A    | C5-C6-N1    | 8.66  | 122.03      | 117.70   |
| 1   | K50   | 204  | C    | O4'-C1'-N1  | 8.58  | 114.50      | 108.50   |
| 1   | L50   | 204  | C    | O4'-C1'-N1  | 8.58  | 114.50      | 108.50   |
| 1   | K50   | 190  | G    | O5'-C5'-C4' | 8.52  | 116.22      | 109.40   |
| 1   | L50   | 190  | G    | O5'-C5'-C4' | 8.52  | 116.22      | 109.40   |
| 1   | K50   | 310  | A    | C4-C5-C6    | -8.30 | 112.85      | 117.00   |
| 1   | K50   | 368  | C    | N3-C2-O2    | -8.30 | 116.09      | 121.90   |
| 1   | L50   | 310  | A    | C4-C5-C6    | -8.30 | 112.85      | 117.00   |
| 1   | L50   | 368  | C    | N3-C2-O2    | -8.30 | 116.09      | 121.90   |
| 1   | K50   | 178  | G    | C1'-O4'-C4' | -8.27 | 103.92      | 109.70   |
| 1   | L50   | 178  | G    | C1'-O4'-C4' | -8.27 | 103.92      | 109.70   |
| 2   | R60   | 63   | G    | P-O3'-C3'   | -8.22 | 109.83      | 119.70   |
| 2   | S60   | 63   | G    | P-O3'-C3'   | -8.22 | 109.83      | 119.70   |
| 2   | R60   | 442  | C    | C2-N1-C1'   | 8.18  | 127.80      | 118.80   |
| 2   | S60   | 442  | C    | C2-N1-C1'   | 8.18  | 127.80      | 118.80   |
| 1   | K50   | 179  | U    | O4'-C1'-N1  | 8.16  | 114.21      | 108.50   |
| 1   | L50   | 179  | U    | O4'-C1'-N1  | 8.16  | 114.21      | 108.50   |
| 1   | K50   | 237  | A    | O5'-C5'-C4' | 8.05  | 115.84      | 109.40   |
| 1   | L50   | 237  | A    | O5'-C5'-C4' | 8.05  | 115.84      | 109.40   |
| 1   | K50   | 310  | A    | N1-C6-N6    | -7.99 | 113.81      | 118.60   |
| 1   | L50   | 310  | A    | N1-C6-N6    | -7.99 | 113.81      | 118.60   |
| 1   | K50   | 1235 | A    | P-O3'-C3'   | -7.93 | 110.19      | 119.70   |
| 1   | L50   | 1235 | A    | P-O3'-C3'   | -7.93 | 110.19      | 119.70   |
| 1   | L50   | 237  | A    | N1-C6-N6    | -7.86 | 113.88      | 118.60   |
| 1   | K50   | 237  | A    | N1-C6-N6    | -7.86 | 113.88      | 118.60   |
| 1   | K50   | 201  | A    | C5-C6-N1    | 7.83  | 121.62      | 117.70   |
| 1   | L50   | 201  | A    | C5-C6-N1    | 7.83  | 121.62      | 117.70   |
| 1   | K50   | 484  | C    | C3'-C2'-C1' | 7.77  | 106.74      | 101.30   |
| 1   | L50   | 484  | C    | C3'-C2'-C1' | 7.77  | 106.74      | 101.30   |
| 2   | R60   | 355  | C    | N3-C2-O2    | -7.76 | 116.47      | 121.90   |
| 2   | S60   | 355  | C    | N3-C2-O2    | -7.76 | 116.47      | 121.90   |
| 49  | ND1   | 103  | ARG  | NE-CZ-NH2   | 7.73  | 126.15      | 119.20   |
| 49  | MD1   | 103  | ARG  | NE-CZ-NH2   | 7.73  | 126.15      | 119.20   |
| 1   | K50   | 205  | C    | C5'-C4'-C3' | -7.71 | 103.66      | 116.00   |
| 1   | L50   | 205  | C    | C5'-C4'-C3' | -7.71 | 103.66      | 116.00   |
| 2   | R60   | 1049 | G    | O5'-C5'-C4' | 7.70  | 115.56      | 109.40   |
| 2   | S60   | 1049 | G    | O5'-C5'-C4' | 7.70  | 115.56      | 109.40   |
| 1   | K50   | 484  | C    | N3-C2-O2    | -7.69 | 116.52      | 121.90   |
| 1   | L50   | 484  | C    | N3-C2-O2    | -7.69 | 116.52      | 121.90   |
| 1   | K50   | 368  | C    | N1-C2-O2    | 7.68  | 123.51      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | L50   | 368  | C    | N1-C2-O2    | 7.68  | 123.51      | 118.90   |
| 1   | K50   | 178  | G    | O3'-P-O5'   | 7.67  | 118.58      | 104.00   |
| 1   | L50   | 178  | G    | O3'-P-O5'   | 7.67  | 118.58      | 104.00   |
| 1   | K50   | 915  | G    | C3'-C2'-C1' | -7.65 | 95.38       | 101.50   |
| 1   | L50   | 915  | G    | C3'-C2'-C1' | -7.65 | 95.38       | 101.50   |
| 1   | K50   | 2    | U    | O5'-C5'-C4' | 7.64  | 115.51      | 109.40   |
| 1   | L50   | 2    | U    | O5'-C5'-C4' | 7.64  | 115.52      | 109.40   |
| 2   | R60   | 1041 | A    | O4'-C1'-N9  | 7.55  | 114.24      | 108.20   |
| 2   | S60   | 1041 | A    | O4'-C1'-N9  | 7.55  | 114.24      | 108.20   |
| 1   | K50   | 202  | G    | O5'-C5'-C4' | 7.53  | 115.42      | 109.40   |
| 1   | L50   | 202  | G    | O5'-C5'-C4' | 7.52  | 115.42      | 109.40   |
| 1   | K50   | 1922 | A    | O4'-C1'-N9  | 7.52  | 114.22      | 108.20   |
| 1   | L50   | 1922 | A    | O4'-C1'-N9  | 7.52  | 114.22      | 108.20   |
| 1   | K50   | 367  | A    | C3'-C2'-C1' | 7.50  | 106.55      | 101.30   |
| 2   | R60   | 67   | C    | C2-N1-C1'   | 7.50  | 127.04      | 118.80   |
| 1   | L50   | 367  | A    | C3'-C2'-C1' | 7.50  | 106.55      | 101.30   |
| 2   | S60   | 67   | C    | C2-N1-C1'   | 7.50  | 127.04      | 118.80   |
| 1   | K50   | 188  | G    | N1-C6-O6    | -7.49 | 115.41      | 119.90   |
| 1   | L50   | 188  | G    | N1-C6-O6    | -7.49 | 115.41      | 119.90   |
| 1   | L50   | 311  | C    | C3'-C2'-C1' | 7.45  | 106.52      | 101.30   |
| 1   | K50   | 311  | C    | C3'-C2'-C1' | 7.45  | 106.52      | 101.30   |
| 1   | L50   | 547  | U    | O4'-C1'-N1  | 7.43  | 113.70      | 108.50   |
| 1   | K50   | 547  | U    | O4'-C1'-N1  | 7.43  | 113.70      | 108.50   |
| 2   | R60   | 83   | G    | O4'-C1'-N9  | -7.41 | 103.32      | 108.50   |
| 2   | S60   | 83   | G    | O4'-C1'-N9  | -7.41 | 103.32      | 108.50   |
| 1   | L50   | 367  | A    | C4-C5-C6    | -7.35 | 113.33      | 117.00   |
| 1   | K50   | 367  | A    | C4-C5-C6    | -7.35 | 113.33      | 117.00   |
| 2   | R60   | 1097 | A    | N9-C4-C5    | -7.35 | 102.86      | 105.80   |
| 2   | S60   | 1097 | A    | N9-C4-C5    | -7.34 | 102.86      | 105.80   |
| 1   | K50   | 1956 | U    | C2-N1-C1'   | 7.34  | 126.51      | 117.70   |
| 1   | L50   | 1956 | U    | C2-N1-C1'   | 7.34  | 126.51      | 117.70   |
| 1   | L50   | 485  | A    | C5-C6-N1    | 7.30  | 121.35      | 117.70   |
| 1   | K50   | 485  | A    | C5-C6-N1    | 7.29  | 121.35      | 117.70   |
| 2   | R60   | 62   | C    | N1-C2-O2    | 7.29  | 123.28      | 118.90   |
| 2   | S60   | 62   | C    | N1-C2-O2    | 7.29  | 123.28      | 118.90   |
| 1   | L50   | 367  | A    | C5-C6-N1    | 7.27  | 121.34      | 117.70   |
| 1   | K50   | 367  | A    | C5-C6-N1    | 7.27  | 121.34      | 117.70   |
| 1   | L50   | 189  | U    | N3-C2-O2    | -7.25 | 117.13      | 122.20   |
| 1   | K50   | 189  | U    | N3-C2-O2    | -7.25 | 117.13      | 122.20   |
| 1   | K50   | 547  | U    | O5'-C5'-C4' | 7.22  | 115.18      | 109.40   |
| 1   | L50   | 547  | U    | O5'-C5'-C4' | 7.22  | 115.18      | 109.40   |
| 1   | L50   | 237  | A    | C5-C6-N1    | 7.18  | 121.29      | 117.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | K50   | 237  | A    | C5-C6-N1    | 7.18  | 121.29      | 117.70   |
| 1   | K50   | 236  | A    | C5-C6-N1    | 7.17  | 121.29      | 117.70   |
| 1   | L50   | 236  | A    | C5-C6-N1    | 7.17  | 121.29      | 117.70   |
| 1   | K50   | 483  | A    | C3'-C2'-C1' | 7.08  | 106.25      | 101.30   |
| 1   | L50   | 483  | A    | C3'-C2'-C1' | 7.08  | 106.25      | 101.30   |
| 1   | K50   | 367  | A    | N1-C6-N6    | -7.06 | 114.37      | 118.60   |
| 1   | L50   | 367  | A    | N1-C6-N6    | -7.06 | 114.36      | 118.60   |
| 1   | K50   | 547  | U    | C5'-C4'-O4' | 7.04  | 116.14      | 109.80   |
| 1   | L50   | 547  | U    | C5'-C4'-O4' | 7.04  | 116.14      | 109.80   |
| 1   | K50   | 1422 | C    | C2-N1-C1'   | 7.01  | 126.52      | 118.80   |
| 1   | L50   | 1422 | C    | C2-N1-C1'   | 7.01  | 126.51      | 118.80   |
| 1   | K50   | 311  | C    | O5'-C5'-C4' | 7.00  | 115.00      | 109.40   |
| 1   | L50   | 311  | C    | O5'-C5'-C4' | 7.00  | 115.00      | 109.40   |
| 1   | K50   | 1717 | A    | P-O3'-C3'   | -6.94 | 111.38      | 119.70   |
| 1   | L50   | 1717 | A    | P-O3'-C3'   | -6.94 | 111.38      | 119.70   |
| 1   | K50   | 205  | C    | N3-C2-O2    | -6.82 | 117.12      | 121.90   |
| 1   | L50   | 205  | C    | N3-C2-O2    | -6.82 | 117.13      | 121.90   |
| 2   | R60   | 794  | G    | P-O3'-C3'   | -6.80 | 111.54      | 119.70   |
| 2   | S60   | 794  | G    | P-O3'-C3'   | -6.80 | 111.54      | 119.70   |
| 1   | K50   | 2268 | A    | P-O3'-C3'   | -6.74 | 111.61      | 119.70   |
| 1   | L50   | 2268 | A    | P-O3'-C3'   | -6.74 | 111.61      | 119.70   |
| 2   | R60   | 1097 | A    | C8-N9-C1'   | -6.73 | 115.59      | 127.70   |
| 2   | S60   | 1097 | A    | C8-N9-C1'   | -6.73 | 115.59      | 127.70   |
| 1   | K50   | 366  | G    | C4-N9-C1'   | -6.71 | 117.78      | 126.50   |
| 1   | L50   | 366  | G    | C4-N9-C1'   | -6.71 | 117.78      | 126.50   |
| 2   | R60   | 1097 | A    | C4-N9-C1'   | 6.67  | 138.30      | 126.30   |
| 2   | S60   | 1097 | A    | C4-N9-C1'   | 6.67  | 138.30      | 126.30   |
| 2   | R60   | 62   | C    | C2-N1-C1'   | 6.65  | 126.11      | 118.80   |
| 2   | S60   | 62   | C    | C2-N1-C1'   | 6.65  | 126.11      | 118.80   |
| 2   | R60   | 869  | G    | N9-C4-C5    | -6.64 | 102.74      | 105.40   |
| 2   | S60   | 869  | G    | N9-C4-C5    | -6.64 | 102.74      | 105.40   |
| 1   | L50   | 976  | C    | N3-C2-O2    | -6.63 | 117.26      | 121.90   |
| 1   | K50   | 976  | C    | N3-C2-O2    | -6.63 | 117.26      | 121.90   |
| 1   | K50   | 179  | U    | O4'-C1'-C2' | -6.61 | 101.66      | 107.60   |
| 1   | L50   | 179  | U    | O4'-C1'-C2' | -6.61 | 101.66      | 107.60   |
| 1   | K50   | 1922 | A    | C3'-C2'-C1' | -6.59 | 96.23       | 101.50   |
| 1   | L50   | 1922 | A    | C3'-C2'-C1' | -6.59 | 96.23       | 101.50   |
| 2   | S60   | 1097 | A    | C6-C5-N7    | -6.57 | 127.70      | 132.30   |
| 1   | K50   | 1224 | A    | P-O3'-C3'   | -6.57 | 111.82      | 119.70   |
| 2   | R60   | 1097 | A    | C6-C5-N7    | -6.57 | 127.70      | 132.30   |
| 1   | L50   | 1224 | A    | P-O3'-C3'   | -6.57 | 111.82      | 119.70   |
| 2   | S60   | 449  | A    | O4'-C1'-N9  | 6.56  | 113.09      | 108.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | R60   | 449  | A    | O4'-C1'-N9  | 6.56  | 113.09      | 108.50   |
| 1   | K50   | 202  | G    | C5'-C4'-C3' | -6.50 | 105.61      | 116.00   |
| 1   | L50   | 202  | G    | C5'-C4'-C3' | -6.50 | 105.61      | 116.00   |
| 1   | K50   | 547  | U    | C3'-C2'-C1' | 6.48  | 105.84      | 101.30   |
| 1   | L50   | 547  | U    | C3'-C2'-C1' | 6.48  | 105.84      | 101.30   |
| 1   | K50   | 237  | A    | C4-C5-C6    | -6.48 | 113.76      | 117.00   |
| 1   | L50   | 237  | A    | C4-C5-C6    | -6.48 | 113.76      | 117.00   |
| 1   | K50   | 724  | C    | O4'-C1'-N1  | 6.43  | 113.00      | 108.50   |
| 1   | L50   | 724  | C    | O4'-C1'-N1  | 6.43  | 113.00      | 108.50   |
| 1   | K50   | 368  | C    | N3-C4-N4    | -6.41 | 113.51      | 118.00   |
| 1   | L50   | 368  | C    | N3-C4-N4    | -6.41 | 113.51      | 118.00   |
| 1   | K50   | 311  | C    | N3-C2-O2    | -6.38 | 117.44      | 121.90   |
| 1   | L50   | 311  | C    | N3-C2-O2    | -6.38 | 117.44      | 121.90   |
| 2   | R60   | 869  | G    | C4-C5-N7    | 6.34  | 113.33      | 110.80   |
| 2   | S60   | 869  | G    | C4-C5-N7    | 6.33  | 113.33      | 110.80   |
| 1   | K50   | 205  | C    | O5'-C5'-C4' | -6.33 | 104.33      | 109.40   |
| 1   | L50   | 205  | C    | O5'-C5'-C4' | -6.33 | 104.33      | 109.40   |
| 2   | R60   | 970  | U    | C2-N1-C1'   | 6.31  | 125.28      | 117.70   |
| 2   | S60   | 970  | U    | C2-N1-C1'   | 6.31  | 125.28      | 117.70   |
| 1   | L50   | 1918 | U    | O5'-C5'-C4' | 6.31  | 114.45      | 109.40   |
| 1   | K50   | 1918 | U    | O5'-C5'-C4' | 6.31  | 114.44      | 109.40   |
| 2   | R60   | 1002 | U    | O5'-C5'-C4' | 6.29  | 114.43      | 109.40   |
| 2   | S60   | 1002 | U    | O5'-C5'-C4' | 6.29  | 114.43      | 109.40   |
| 1   | K50   | 547  | U    | C1'-O4'-C4' | -6.27 | 104.89      | 109.90   |
| 1   | L50   | 547  | U    | C1'-O4'-C4' | -6.27 | 104.89      | 109.90   |
| 1   | K50   | 204  | C    | N3-C2-O2    | -6.27 | 117.51      | 121.90   |
| 1   | L50   | 204  | C    | N3-C2-O2    | -6.26 | 117.52      | 121.90   |
| 1   | K50   | 2480 | C    | C2-N1-C1'   | 6.25  | 125.67      | 118.80   |
| 1   | L50   | 2480 | C    | C2-N1-C1'   | 6.25  | 125.67      | 118.80   |
| 2   | R60   | 62   | C    | N3-C2-O2    | -6.24 | 117.53      | 121.90   |
| 2   | S60   | 62   | C    | N3-C2-O2    | -6.24 | 117.53      | 121.90   |
| 2   | R60   | 825  | U    | C2-N1-C1'   | 6.23  | 125.17      | 117.70   |
| 2   | S60   | 825  | U    | C2-N1-C1'   | 6.23  | 125.17      | 117.70   |
| 1   | L50   | 201  | A    | C4-C5-C6    | -6.22 | 113.89      | 117.00   |
| 1   | K50   | 201  | A    | C4-C5-C6    | -6.22 | 113.89      | 117.00   |
| 24  | KEE   | 82   | MET  | CB-CG-SD    | 6.21  | 131.31      | 112.70   |
| 24  | LEE   | 82   | MET  | CB-CG-SD    | 6.21  | 131.31      | 112.70   |
| 2   | S60   | 562  | G    | O5'-C5'-C4' | 6.20  | 114.36      | 109.40   |
| 2   | R60   | 562  | G    | O5'-C5'-C4' | 6.20  | 114.36      | 109.40   |
| 2   | R60   | 855  | G    | N9-C1'-C2'  | 6.16  | 118.77      | 112.00   |
| 2   | R60   | 144  | G    | C4-N9-C1'   | 6.16  | 134.50      | 126.50   |
| 2   | R60   | 442  | C    | C6-N1-C1'   | -6.16 | 113.41      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | S60   | 144  | G    | C4-N9-C1'   | 6.16  | 134.50      | 126.50   |
| 2   | S60   | 442  | C    | C6-N1-C1'   | -6.16 | 113.41      | 120.80   |
| 2   | S60   | 855  | G    | N9-C1'-C2'  | 6.16  | 118.77      | 112.00   |
| 2   | R60   | 1097 | A    | N3-C4-N9    | 6.15  | 132.32      | 127.40   |
| 2   | S60   | 1097 | A    | N3-C4-N9    | 6.15  | 132.32      | 127.40   |
| 1   | K50   | 367  | A    | N9-C1'-C2'  | -6.14 | 105.24      | 112.00   |
| 1   | L50   | 367  | A    | N9-C1'-C2'  | -6.14 | 105.24      | 112.00   |
| 1   | K50   | 484  | C    | N3-C4-C5    | 6.12  | 124.35      | 121.90   |
| 1   | L50   | 484  | C    | N3-C4-C5    | 6.12  | 124.35      | 121.90   |
| 2   | R60   | 1313 | A    | O5'-C5'-C4' | 6.10  | 114.28      | 109.40   |
| 2   | R60   | 363  | C    | O5'-C5'-C4' | 6.09  | 114.28      | 109.40   |
| 2   | S60   | 363  | C    | O5'-C5'-C4' | 6.09  | 114.28      | 109.40   |
| 2   | S60   | 1313 | A    | O5'-C5'-C4' | 6.09  | 114.28      | 109.40   |
| 2   | R60   | 1275 | C    | C2-N1-C1'   | -6.06 | 112.13      | 118.80   |
| 2   | S60   | 1275 | C    | C2-N1-C1'   | -6.06 | 112.13      | 118.80   |
| 2   | R60   | 1222 | C    | O5'-C5'-C4' | 6.05  | 114.24      | 109.40   |
| 2   | S60   | 1222 | C    | O5'-C5'-C4' | 6.05  | 114.24      | 109.40   |
| 1   | K50   | 188  | G    | O4'-C1'-N9  | 6.01  | 112.71      | 108.50   |
| 1   | L50   | 188  | G    | O4'-C1'-N9  | 6.01  | 112.71      | 108.50   |
| 2   | R60   | 960  | U    | C5-C4-O4    | -6.01 | 122.30      | 125.90   |
| 2   | S60   | 960  | U    | C5-C4-O4    | -6.01 | 122.30      | 125.90   |
| 2   | S60   | 1097 | A    | O4'-C1'-N9  | -5.97 | 104.32      | 108.50   |
| 2   | R60   | 1097 | A    | O4'-C1'-N9  | -5.97 | 104.32      | 108.50   |
| 39  | KQ0   | 173  | ARG  | NE-CZ-NH2   | 5.96  | 124.57      | 119.20   |
| 39  | LQ0   | 173  | ARG  | NE-CZ-NH2   | 5.96  | 124.57      | 119.20   |
| 2   | R60   | 859  | G    | O5'-C5'-C4' | 5.96  | 114.17      | 109.40   |
| 2   | S60   | 859  | G    | O5'-C5'-C4' | 5.96  | 114.17      | 109.40   |
| 2   | R60   | 134  | G    | N3-C4-N9    | 5.94  | 129.57      | 126.00   |
| 2   | S60   | 134  | G    | N3-C4-N9    | 5.94  | 129.57      | 126.00   |
| 1   | K50   | 311  | C    | C2'-C3'-O3' | 5.92  | 123.17      | 113.70   |
| 1   | L50   | 311  | C    | C2'-C3'-O3' | 5.92  | 123.17      | 113.70   |
| 2   | R60   | 388  | G    | O4'-C1'-N9  | -5.91 | 104.36      | 108.50   |
| 2   | S60   | 388  | G    | O4'-C1'-N9  | -5.91 | 104.36      | 108.50   |
| 1   | K50   | 2480 | C    | C6-N1-C2    | -5.88 | 117.95      | 120.30   |
| 1   | L50   | 2480 | C    | C6-N1-C2    | -5.88 | 117.95      | 120.30   |
| 1   | K50   | 666  | A    | P-O3'-C3'   | -5.87 | 112.65      | 119.70   |
| 2   | R60   | 67   | C    | N1-C2-O2    | 5.87  | 122.42      | 118.90   |
| 2   | R60   | 1017 | A    | O4'-C1'-N9  | 5.87  | 112.61      | 108.50   |
| 1   | L50   | 666  | A    | P-O3'-C3'   | -5.87 | 112.65      | 119.70   |
| 2   | S60   | 67   | C    | N1-C2-O2    | 5.87  | 122.42      | 118.90   |
| 2   | S60   | 1017 | A    | O4'-C1'-N9  | 5.87  | 112.61      | 108.50   |
| 18  | KAA   | 49   | HIS  | CB-CG-CD2   | -5.87 | 123.57      | 131.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | LAA   | 49   | HIS  | CB-CG-CD2   | -5.87 | 123.57      | 131.20   |
| 1   | K50   | 546  | G    | N1-C6-O6    | -5.86 | 116.38      | 119.90   |
| 1   | L50   | 546  | G    | N1-C6-O6    | -5.86 | 116.38      | 119.90   |
| 1   | K50   | 369  | U    | N1-C2-N3    | 5.86  | 118.42      | 114.90   |
| 1   | L50   | 369  | U    | N1-C2-N3    | 5.86  | 118.42      | 114.90   |
| 1   | L50   | 368  | C    | O4'-C1'-N1  | 5.85  | 112.60      | 108.50   |
| 1   | K50   | 368  | C    | O4'-C1'-N1  | 5.85  | 112.60      | 108.50   |
| 1   | K50   | 201  | A    | C3'-C2'-C1' | -5.85 | 96.82       | 101.50   |
| 1   | L50   | 201  | A    | C3'-C2'-C1' | -5.85 | 96.82       | 101.50   |
| 1   | K50   | 2586 | U    | O4'-C1'-N1  | -5.84 | 104.42      | 108.50   |
| 1   | L50   | 2586 | U    | O4'-C1'-N1  | -5.84 | 104.42      | 108.50   |
| 2   | R60   | 970  | U    | O4'-C1'-N1  | -5.83 | 104.42      | 108.50   |
| 2   | S60   | 83   | G    | C8-N9-C1'   | -5.83 | 119.43      | 127.00   |
| 2   | S60   | 970  | U    | O4'-C1'-N1  | -5.83 | 104.42      | 108.50   |
| 2   | R60   | 83   | G    | C8-N9-C1'   | -5.82 | 119.43      | 127.00   |
| 2   | R60   | 442  | C    | N1-C2-O2    | 5.82  | 122.39      | 118.90   |
| 2   | S60   | 442  | C    | N1-C2-O2    | 5.82  | 122.39      | 118.90   |
| 1   | K50   | 1936 | U    | O4'-C1'-N1  | 5.80  | 112.56      | 108.50   |
| 1   | L50   | 1936 | U    | O4'-C1'-N1  | 5.80  | 112.56      | 108.50   |
| 1   | K50   | 205  | C    | O4'-C4'-C3' | 5.80  | 109.80      | 104.00   |
| 1   | L50   | 205  | C    | O4'-C4'-C3' | 5.80  | 109.80      | 104.00   |
| 2   | R60   | 83   | G    | N9-C4-C5    | -5.80 | 103.08      | 105.40   |
| 2   | R60   | 941  | C    | C2-N1-C1'   | 5.80  | 125.18      | 118.80   |
| 2   | S60   | 941  | C    | C2-N1-C1'   | 5.80  | 125.18      | 118.80   |
| 2   | S60   | 83   | G    | N9-C4-C5    | -5.79 | 103.08      | 105.40   |
| 1   | K50   | 900  | A    | O5'-C5'-C4' | 5.77  | 114.01      | 109.40   |
| 1   | L50   | 900  | A    | O5'-C5'-C4' | 5.77  | 114.01      | 109.40   |
| 1   | K50   | 2299 | C    | P-O3'-C3'   | -5.76 | 112.79      | 119.70   |
| 1   | L50   | 236  | A    | C4-C5-C6    | -5.76 | 114.12      | 117.00   |
| 1   | L50   | 2299 | C    | P-O3'-C3'   | -5.76 | 112.79      | 119.70   |
| 1   | K50   | 236  | A    | C4-C5-C6    | -5.76 | 114.12      | 117.00   |
| 2   | R60   | 144  | G    | C8-N9-C1'   | -5.76 | 119.52      | 127.00   |
| 1   | L50   | 2559 | G    | P-O3'-C3'   | -5.76 | 112.79      | 119.70   |
| 2   | S60   | 144  | G    | C8-N9-C1'   | -5.76 | 119.52      | 127.00   |
| 1   | K50   | 2559 | G    | P-O3'-C3'   | -5.75 | 112.79      | 119.70   |
| 1   | K50   | 205  | C    | C3'-C2'-C1' | 5.75  | 105.32      | 101.30   |
| 1   | L50   | 205  | C    | C3'-C2'-C1' | 5.75  | 105.32      | 101.30   |
| 1   | K50   | 202  | G    | C5'-C4'-O4' | 5.74  | 114.96      | 109.80   |
| 49  | ND1   | 27   | ILE  | CA-C-N      | 5.74  | 130.57      | 120.87   |
| 49  | ND1   | 27   | ILE  | C-N-CA      | 5.74  | 130.57      | 120.87   |
| 1   | L50   | 202  | G    | C5'-C4'-O4' | 5.74  | 114.96      | 109.80   |
| 49  | MD1   | 27   | ILE  | CA-C-N      | 5.74  | 130.57      | 120.87   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 49  | MD1   | 27   | ILE  | C-N-CA      | 5.74  | 130.57      | 120.87   |
| 1   | K50   | 2480 | C    | N1-C2-O2    | 5.74  | 122.34      | 118.90   |
| 1   | L50   | 2480 | C    | N1-C2-O2    | 5.73  | 122.34      | 118.90   |
| 1   | L50   | 485  | A    | C4-C5-C6    | -5.73 | 114.13      | 117.00   |
| 1   | K50   | 485  | A    | C4-C5-C6    | -5.73 | 114.14      | 117.00   |
| 1   | K50   | 1234 | U    | C2-N1-C1'   | 5.72  | 124.57      | 117.70   |
| 1   | L50   | 1234 | U    | C2-N1-C1'   | 5.72  | 124.57      | 117.70   |
| 2   | R60   | 524  | G    | O5'-C5'-C4' | 5.72  | 113.97      | 109.40   |
| 2   | S60   | 524  | G    | O5'-C5'-C4' | 5.72  | 113.97      | 109.40   |
| 78  | RF0   | 127  | ARG  | NE-CZ-NH2   | 5.72  | 124.34      | 119.20   |
| 78  | SF0   | 127  | ARG  | NE-CZ-NH2   | 5.72  | 124.34      | 119.20   |
| 2   | R60   | 137  | A    | N9-C1'-C2'  | 5.71  | 118.29      | 112.00   |
| 2   | S60   | 137  | A    | N9-C1'-C2'  | 5.71  | 118.29      | 112.00   |
| 2   | R60   | 1223 | C    | O5'-C5'-C4' | 5.70  | 113.96      | 109.40   |
| 2   | S60   | 1223 | C    | O5'-C5'-C4' | 5.70  | 113.96      | 109.40   |
| 1   | L50   | 483  | A    | C4-C5-C6    | -5.69 | 114.15      | 117.00   |
| 1   | K50   | 483  | A    | C4-C5-C6    | -5.69 | 114.16      | 117.00   |
| 1   | K50   | 204  | C    | N1-C2-O2    | 5.69  | 122.31      | 118.90   |
| 2   | R60   | 761  | G    | O5'-C5'-C4' | 5.69  | 113.95      | 109.40   |
| 2   | S60   | 761  | G    | O5'-C5'-C4' | 5.69  | 113.95      | 109.40   |
| 1   | L50   | 204  | C    | N1-C2-O2    | 5.69  | 122.31      | 118.90   |
| 1   | K50   | 2558 | A    | P-O3'-C3'   | -5.66 | 112.91      | 119.70   |
| 1   | L50   | 2558 | A    | P-O3'-C3'   | -5.66 | 112.91      | 119.70   |
| 1   | L50   | 1443 | C    | P-O3'-C3'   | -5.64 | 112.93      | 119.70   |
| 1   | K50   | 1443 | C    | P-O3'-C3'   | -5.64 | 112.93      | 119.70   |
| 33  | KL0   | 12   | PHE  | CA-C-N      | 5.63  | 127.83      | 120.28   |
| 33  | KL0   | 12   | PHE  | C-N-CA      | 5.63  | 127.83      | 120.28   |
| 33  | LL0   | 12   | PHE  | CA-C-N      | 5.63  | 127.83      | 120.28   |
| 33  | LL0   | 12   | PHE  | C-N-CA      | 5.63  | 127.83      | 120.28   |
| 1   | K50   | 484  | C    | C2-N3-C4    | -5.63 | 117.08      | 119.90   |
| 1   | L50   | 484  | C    | C2-N3-C4    | -5.63 | 117.08      | 119.90   |
| 2   | R60   | 355  | C    | C2-N1-C1'   | 5.63  | 124.99      | 118.80   |
| 2   | S60   | 355  | C    | C2-N1-C1'   | 5.63  | 124.99      | 118.80   |
| 1   | K50   | 1236 | U    | P-O3'-C3'   | -5.62 | 112.95      | 119.70   |
| 1   | L50   | 1236 | U    | P-O3'-C3'   | -5.62 | 112.95      | 119.70   |
| 1   | K50   | 923  | G    | C4-N9-C1'   | 5.62  | 133.80      | 126.50   |
| 1   | L50   | 923  | G    | C4-N9-C1'   | 5.62  | 133.80      | 126.50   |
| 2   | S60   | 512  | C    | O5'-C5'-C4' | 5.61  | 113.89      | 109.40   |
| 2   | R60   | 512  | C    | O5'-C5'-C4' | 5.61  | 113.89      | 109.40   |
| 2   | R60   | 1026 | U    | C2-N1-C1'   | -5.61 | 110.97      | 117.70   |
| 2   | S60   | 1026 | U    | C2-N1-C1'   | -5.61 | 110.97      | 117.70   |
| 1   | K50   | 923  | G    | C8-N9-C1'   | -5.60 | 119.72      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | R60   | 1090 | C    | O5'-C5'-C4' | 5.60  | 113.88      | 109.40   |
| 1   | L50   | 923  | G    | C8-N9-C1'   | -5.60 | 119.72      | 127.00   |
| 2   | S60   | 1090 | C    | O5'-C5'-C4' | 5.60  | 113.88      | 109.40   |
| 1   | K50   | 548  | G    | C4'-C3'-C2' | -5.60 | 97.00       | 102.60   |
| 1   | L50   | 548  | G    | C4'-C3'-C2' | -5.60 | 97.00       | 102.60   |
| 2   | R60   | 1060 | G    | C5-C6-N1    | 5.57  | 114.28      | 111.50   |
| 2   | S60   | 1060 | G    | C5-C6-N1    | 5.57  | 114.28      | 111.50   |
| 2   | S60   | 1019 | C    | N3-C2-O2    | -5.56 | 118.01      | 121.90   |
| 2   | R60   | 1019 | C    | N3-C2-O2    | -5.56 | 118.01      | 121.90   |
| 1   | L50   | 547  | U    | N3-C2-O2    | -5.56 | 118.31      | 122.20   |
| 1   | K50   | 547  | U    | N3-C2-O2    | -5.56 | 118.31      | 122.20   |
| 1   | L50   | 2018 | G    | N3-C4-N9    | -5.56 | 122.67      | 126.00   |
| 1   | K50   | 2018 | G    | N3-C4-N9    | -5.55 | 122.67      | 126.00   |
| 2   | S60   | 473  | G    | C4-N9-C1'   | 5.55  | 133.71      | 126.50   |
| 2   | R60   | 473  | G    | C4-N9-C1'   | 5.55  | 133.71      | 126.50   |
| 2   | S60   | 1165 | C    | N1-C2-O2    | 5.54  | 122.23      | 118.90   |
| 2   | R60   | 1165 | C    | N1-C2-O2    | 5.54  | 122.22      | 118.90   |
| 2   | R60   | 569  | G    | C4-N9-C1'   | -5.54 | 119.30      | 126.50   |
| 2   | S60   | 569  | G    | C4-N9-C1'   | -5.54 | 119.30      | 126.50   |
| 2   | R60   | 820  | G    | C4-N9-C1'   | 5.53  | 133.69      | 126.50   |
| 2   | S60   | 820  | G    | C4-N9-C1'   | 5.53  | 133.69      | 126.50   |
| 2   | R60   | 61   | G    | N1-C2-N2    | -5.52 | 111.23      | 116.20   |
| 2   | S60   | 61   | G    | N1-C2-N2    | -5.52 | 111.23      | 116.20   |
| 1   | K50   | 1897 | G    | O5'-C5'-C4' | 5.51  | 113.81      | 109.40   |
| 1   | L50   | 1897 | G    | O5'-C5'-C4' | 5.51  | 113.81      | 109.40   |
| 2   | R60   | 833  | A    | O5'-C5'-C4' | 5.50  | 113.80      | 109.40   |
| 8   | B     | 22   | ILE  | CB-CA-C     | 5.50  | 116.68      | 110.41   |
| 2   | S60   | 833  | A    | O5'-C5'-C4' | 5.50  | 113.80      | 109.40   |
| 8   | A     | 22   | ILE  | CB-CA-C     | 5.50  | 116.68      | 110.41   |
| 1   | K50   | 202  | G    | N9-C1'-C2'  | -5.49 | 105.96      | 112.00   |
| 1   | L50   | 202  | G    | N9-C1'-C2'  | -5.49 | 105.96      | 112.00   |
| 2   | S60   | 1138 | U    | C2-N1-C1'   | 5.48  | 124.27      | 117.70   |
| 2   | R60   | 1138 | U    | C2-N1-C1'   | 5.48  | 124.27      | 117.70   |
| 2   | R60   | 83   | G    | N3-C4-N9    | 5.48  | 129.28      | 126.00   |
| 2   | S60   | 83   | G    | N3-C4-N9    | 5.48  | 129.28      | 126.00   |
| 1   | K50   | 203  | U    | N3-C2-O2    | -5.47 | 118.37      | 122.20   |
| 1   | L50   | 203  | U    | N3-C2-O2    | -5.47 | 118.37      | 122.20   |
| 1   | K50   | 2480 | C    | N3-C2-O2    | -5.46 | 118.08      | 121.90   |
| 1   | L50   | 2480 | C    | N3-C2-O2    | -5.46 | 118.08      | 121.90   |
| 1   | K50   | 1422 | C    | C6-N1-C1'   | -5.45 | 114.27      | 120.80   |
| 1   | L50   | 1422 | C    | C6-N1-C1'   | -5.45 | 114.27      | 120.80   |
| 2   | R60   | 280  | G    | O5'-C5'-C4' | 5.44  | 113.75      | 109.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | S60   | 280  | G    | O5'-C5'-C4' | 5.44  | 113.75      | 109.40   |
| 2   | R60   | 1060 | G    | N3-C4-N9    | 5.43  | 129.26      | 126.00   |
| 2   | S60   | 1060 | G    | N3-C4-N9    | 5.43  | 129.26      | 126.00   |
| 7   | L70   | 49   | A    | O4'-C1'-N9  | 5.43  | 112.30      | 108.50   |
| 7   | K70   | 49   | A    | O4'-C1'-N9  | 5.42  | 112.30      | 108.50   |
| 2   | R60   | 746  | G    | O5'-C5'-C4' | 5.42  | 113.73      | 109.40   |
| 2   | S60   | 746  | G    | O5'-C5'-C4' | 5.42  | 113.73      | 109.40   |
| 1   | K50   | 2002 | C    | N1-C2-O2    | -5.42 | 115.65      | 118.90   |
| 2   | R60   | 871  | C    | P-O3'-C3'   | -5.42 | 113.20      | 119.70   |
| 2   | S60   | 871  | C    | P-O3'-C3'   | -5.42 | 113.20      | 119.70   |
| 1   | L50   | 2002 | C    | N1-C2-O2    | -5.42 | 115.65      | 118.90   |
| 49  | ND1   | 59   | LYS  | N-CA-CB     | -5.40 | 104.09      | 111.65   |
| 49  | MD1   | 59   | LYS  | N-CA-CB     | -5.40 | 104.09      | 111.65   |
| 2   | R60   | 1000 | C    | N3-C2-O2    | -5.39 | 118.12      | 121.90   |
| 2   | S60   | 1000 | C    | N3-C2-O2    | -5.39 | 118.12      | 121.90   |
| 2   | R60   | 1191 | C    | O5'-C5'-C4' | 5.37  | 113.70      | 109.40   |
| 2   | S60   | 1191 | C    | O5'-C5'-C4' | 5.37  | 113.70      | 109.40   |
| 19  | KB0   | 76   | GLU  | OE1-CD-OE2  | 5.36  | 135.77      | 122.90   |
| 19  | LB0   | 76   | GLU  | OE1-CD-OE2  | 5.36  | 135.77      | 122.90   |
| 1   | K50   | 549  | C    | N3-C2-O2    | -5.36 | 118.15      | 121.90   |
| 1   | L50   | 549  | C    | N3-C2-O2    | -5.36 | 118.15      | 121.90   |
| 1   | K50   | 923  | G    | N3-C4-N9    | 5.36  | 129.21      | 126.00   |
| 1   | L50   | 923  | G    | N3-C4-N9    | 5.36  | 129.22      | 126.00   |
| 1   | K50   | 178  | G    | O4'-C4'-C3' | 5.35  | 110.38      | 106.10   |
| 24  | KEE   | 82   | MET  | N-CA-C      | -5.35 | 100.68      | 109.40   |
| 1   | L50   | 178  | G    | O4'-C4'-C3' | 5.35  | 110.38      | 106.10   |
| 24  | LEE   | 82   | MET  | N-CA-C      | -5.35 | 100.68      | 109.40   |
| 1   | K50   | 178  | G    | C4'-C3'-C2' | -5.35 | 97.25       | 102.60   |
| 1   | L50   | 178  | G    | C4'-C3'-C2' | -5.35 | 97.25       | 102.60   |
| 1   | K50   | 237  | A    | C5'-C4'-O4' | 5.35  | 114.61      | 109.80   |
| 2   | R60   | 67   | C    | C6-N1-C1'   | -5.35 | 114.38      | 120.80   |
| 1   | L50   | 237  | A    | C5'-C4'-O4' | 5.35  | 114.61      | 109.80   |
| 2   | S60   | 67   | C    | C6-N1-C1'   | -5.35 | 114.38      | 120.80   |
| 1   | L50   | 1922 | A    | C1'-O4'-C4' | -5.34 | 105.96      | 109.70   |
| 1   | K50   | 1922 | A    | C1'-O4'-C4' | -5.34 | 105.96      | 109.70   |
| 23  | KE0   | 58   | TYR  | N-CA-C      | -5.34 | 106.95      | 112.93   |
| 23  | LE0   | 58   | TYR  | N-CA-C      | -5.34 | 106.95      | 112.93   |
| 8   | B     | 22   | ILE  | N-CA-C      | 5.33  | 116.41      | 107.18   |
| 8   | A     | 22   | ILE  | N-CA-C      | 5.33  | 116.41      | 107.18   |
| 17  | LA0   | 180  | TYR  | CB-CG-CD2   | -5.32 | 112.81      | 120.80   |
| 17  | LA02  | 180  | TYR  | CB-CG-CD2   | -5.32 | 112.82      | 120.80   |
| 2   | S60   | 82   | C    | N3-C2-O2    | -5.32 | 118.17      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | R60   | 82   | C    | N3-C2-O2    | -5.32 | 118.17      | 121.90   |
| 1   | K50   | 976  | C    | N1-C2-O2    | 5.32  | 122.09      | 118.90   |
| 1   | L50   | 976  | C    | N1-C2-O2    | 5.32  | 122.09      | 118.90   |
| 1   | K50   | 368  | C    | O5'-C5'-C4' | -5.31 | 105.15      | 109.40   |
| 1   | L50   | 368  | C    | O5'-C5'-C4' | -5.31 | 105.15      | 109.40   |
| 2   | S60   | 961  | G    | O4'-C1'-N9  | 5.31  | 112.22      | 108.50   |
| 1   | K50   | 1162 | U    | C2-N1-C1'   | 5.31  | 124.07      | 117.70   |
| 2   | R60   | 961  | G    | O4'-C1'-N9  | 5.31  | 112.22      | 108.50   |
| 1   | L50   | 1162 | U    | C2-N1-C1'   | 5.31  | 124.07      | 117.70   |
| 50  | RA0   | 94   | ILE  | N-CA-C      | -5.31 | 107.65      | 112.96   |
| 50  | SA0   | 94   | ILE  | N-CA-C      | -5.31 | 107.65      | 112.96   |
| 1   | K50   | 1894 | G    | O4'-C1'-N9  | -5.29 | 104.80      | 108.50   |
| 1   | L50   | 1894 | G    | O4'-C1'-N9  | -5.29 | 104.80      | 108.50   |
| 1   | K50   | 2481 | U    | N3-C4-O4    | -5.29 | 115.70      | 119.40   |
| 1   | L50   | 2481 | U    | N3-C4-O4    | -5.29 | 115.70      | 119.40   |
| 1   | K50   | 204  | C    | C5'-C4'-O4' | 5.28  | 114.55      | 109.80   |
| 1   | L50   | 204  | C    | C5'-C4'-O4' | 5.27  | 114.55      | 109.80   |
| 1   | L50   | 190  | G    | C8-N9-C4    | -5.27 | 104.29      | 106.40   |
| 1   | K50   | 190  | G    | C8-N9-C4    | -5.27 | 104.29      | 106.40   |
| 1   | K50   | 972  | C    | O5'-C5'-C4' | 5.26  | 113.61      | 109.40   |
| 1   | L50   | 972  | C    | O5'-C5'-C4' | 5.26  | 113.61      | 109.40   |
| 2   | R60   | 67   | C    | O4'-C1'-N1  | -5.25 | 104.82      | 108.50   |
| 2   | S60   | 67   | C    | O4'-C1'-N1  | -5.25 | 104.82      | 108.50   |
| 2   | R60   | 927  | G    | C5-C6-O6    | 5.25  | 131.75      | 128.60   |
| 2   | S60   | 927  | G    | C5-C6-O6    | 5.25  | 131.75      | 128.60   |
| 1   | K50   | 205  | C    | N3-C4-C5    | 5.24  | 124.00      | 121.90   |
| 1   | L50   | 205  | C    | N3-C4-C5    | 5.24  | 124.00      | 121.90   |
| 1   | K50   | 188  | G    | N9-C1'-C2'  | -5.23 | 106.25      | 112.00   |
| 1   | K50   | 188  | G    | O5'-C5'-C4' | -5.23 | 105.22      | 109.40   |
| 1   | L50   | 188  | G    | N9-C1'-C2'  | -5.23 | 106.25      | 112.00   |
| 2   | R60   | 569  | G    | C8-N9-C1'   | 5.23  | 133.80      | 127.00   |
| 1   | L50   | 188  | G    | O5'-C5'-C4' | -5.23 | 105.22      | 109.40   |
| 2   | S60   | 569  | G    | C8-N9-C1'   | 5.23  | 133.80      | 127.00   |
| 1   | K50   | 808  | C    | N3-C2-O2    | -5.22 | 118.24      | 121.90   |
| 1   | L50   | 808  | C    | N3-C2-O2    | -5.22 | 118.24      | 121.90   |
| 1   | K50   | 923  | G    | C6-C5-N7    | -5.21 | 127.27      | 130.40   |
| 1   | L50   | 923  | G    | C6-C5-N7    | -5.21 | 127.27      | 130.40   |
| 2   | R60   | 869  | G    | C6-C5-N7    | -5.21 | 127.27      | 130.40   |
| 2   | S60   | 869  | G    | C6-C5-N7    | -5.21 | 127.28      | 130.40   |
| 1   | K50   | 369  | U    | N3-C2-O2    | -5.20 | 118.56      | 122.20   |
| 1   | L50   | 369  | U    | N3-C2-O2    | -5.20 | 118.56      | 122.20   |
| 2   | R60   | 1275 | C    | C6-N1-C1'   | 5.20  | 127.04      | 120.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | S60   | 1275 | C    | C6-N1-C1'   | 5.20  | 127.04      | 120.80   |
| 1   | K50   | 190  | G    | N7-C8-N9    | 5.18  | 115.69      | 113.10   |
| 1   | K50   | 2038 | A    | N9-C1'-C2'  | 5.18  | 117.70      | 112.00   |
| 1   | L50   | 190  | G    | N7-C8-N9    | 5.18  | 115.69      | 113.10   |
| 1   | L50   | 2038 | A    | N9-C1'-C2'  | 5.18  | 117.70      | 112.00   |
| 1   | K50   | 189  | U    | O4'-C1'-C2' | -5.17 | 102.95      | 107.60   |
| 1   | L50   | 189  | U    | O4'-C1'-C2' | -5.17 | 102.95      | 107.60   |
| 2   | S60   | 980  | G    | N1-C6-O6    | -5.15 | 116.81      | 119.90   |
| 2   | R60   | 980  | G    | N1-C6-O6    | -5.15 | 116.81      | 119.90   |
| 1   | K50   | 547  | U    | C5-C6-N1    | -5.15 | 120.13      | 122.70   |
| 2   | S60   | 970  | U    | C6-N1-C1'   | -5.15 | 113.99      | 121.20   |
| 2   | R60   | 970  | U    | C6-N1-C1'   | -5.15 | 114.00      | 121.20   |
| 1   | L50   | 547  | U    | C5-C6-N1    | -5.15 | 120.13      | 122.70   |
| 1   | K50   | 203  | U    | C5-C6-N1    | -5.14 | 120.13      | 122.70   |
| 2   | R60   | 58   | U    | O4'-C1'-N1  | -5.14 | 104.90      | 108.50   |
| 1   | K50   | 310  | A    | C5'-C4'-O4' | 5.14  | 114.43      | 109.80   |
| 1   | L50   | 203  | U    | C5-C6-N1    | -5.14 | 120.13      | 122.70   |
| 1   | L50   | 310  | A    | C5'-C4'-O4' | 5.14  | 114.43      | 109.80   |
| 2   | S60   | 58   | U    | O4'-C1'-N1  | -5.14 | 104.90      | 108.50   |
| 1   | L50   | 450  | C    | C6-N1-C2    | -5.13 | 118.25      | 120.30   |
| 1   | K50   | 450  | C    | C6-N1-C2    | -5.13 | 118.25      | 120.30   |
| 2   | R60   | 28   | G    | O5'-C5'-C4' | 5.13  | 113.50      | 109.40   |
| 2   | S60   | 28   | G    | O5'-C5'-C4' | 5.13  | 113.50      | 109.40   |
| 2   | R60   | 465  | U    | O5'-C5'-C4' | 5.12  | 113.50      | 109.40   |
| 2   | S60   | 465  | U    | O5'-C5'-C4' | 5.12  | 113.50      | 109.40   |
| 1   | K50   | 188  | G    | C5-C6-N1    | 5.12  | 114.06      | 111.50   |
| 1   | K50   | 1940 | C    | C2-N1-C1'   | -5.12 | 113.17      | 118.80   |
| 1   | L50   | 1940 | C    | C2-N1-C1'   | -5.12 | 113.17      | 118.80   |
| 1   | L50   | 188  | G    | C5-C6-N1    | 5.12  | 114.06      | 111.50   |
| 1   | K50   | 484  | C    | N1-C2-O2    | 5.12  | 121.97      | 118.90   |
| 1   | L50   | 484  | C    | N1-C2-O2    | 5.12  | 121.97      | 118.90   |
| 1   | K50   | 1956 | U    | C6-N1-C1'   | -5.11 | 114.04      | 121.20   |
| 2   | R60   | 914  | U    | O5'-C5'-C4' | 5.11  | 113.49      | 109.40   |
| 1   | L50   | 1956 | U    | C6-N1-C1'   | -5.11 | 114.04      | 121.20   |
| 2   | S60   | 914  | U    | O5'-C5'-C4' | 5.11  | 113.49      | 109.40   |
| 29  | KHH   | 108  | TYR  | CB-CA-C     | 5.10  | 119.67      | 111.36   |
| 29  | LHH   | 108  | TYR  | CB-CA-C     | 5.10  | 119.67      | 111.36   |
| 2   | R60   | 1097 | A    | O5'-C5'-C4' | 5.09  | 113.47      | 109.40   |
| 2   | S60   | 1097 | A    | O5'-C5'-C4' | 5.09  | 113.47      | 109.40   |
| 1   | K50   | 1190 | C    | C2-N1-C1'   | 5.07  | 124.38      | 118.80   |
| 1   | L50   | 1190 | C    | C2-N1-C1'   | 5.07  | 124.38      | 118.80   |
| 2   | R60   | 172  | U    | O4'-C1'-N1  | 5.07  | 112.26      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | S60   | 172  | U    | O4'-C1'-N1  | 5.07  | 112.26      | 108.20   |
| 2   | R60   | 927  | G    | N1-C6-O6    | -5.07 | 116.86      | 119.90   |
| 2   | R60   | 1148 | A    | O5'-C5'-C4' | 5.07  | 113.45      | 109.40   |
| 2   | S60   | 927  | G    | N1-C6-O6    | -5.07 | 116.86      | 119.90   |
| 2   | S60   | 1148 | A    | O5'-C5'-C4' | 5.07  | 113.45      | 109.40   |
| 2   | R60   | 67   | C    | N3-C2-O2    | -5.07 | 118.35      | 121.90   |
| 2   | R60   | 1022 | C    | O5'-C5'-C4' | 5.07  | 113.45      | 109.40   |
| 2   | S60   | 67   | C    | N3-C2-O2    | -5.07 | 118.35      | 121.90   |
| 2   | S60   | 1022 | C    | O5'-C5'-C4' | 5.07  | 113.45      | 109.40   |
| 2   | R60   | 62   | C    | C6-N1-C1'   | -5.06 | 114.73      | 120.80   |
| 2   | S60   | 62   | C    | C6-N1-C1'   | -5.06 | 114.73      | 120.80   |
| 1   | K50   | 810  | U    | O5'-C5'-C4' | -5.05 | 105.36      | 109.40   |
| 1   | L50   | 810  | U    | O5'-C5'-C4' | -5.05 | 105.36      | 109.40   |
| 2   | S60   | 946  | C    | N3-C4-C5    | 5.04  | 123.92      | 121.90   |
| 2   | R60   | 946  | C    | N3-C4-C5    | 5.04  | 123.92      | 121.90   |
| 78  | SF0   | 127  | ARG  | CD-NE-CZ    | 5.04  | 131.46      | 124.40   |
| 7   | K70   | 1    | A    | N9-C1'-C2'  | 5.04  | 117.55      | 112.00   |
| 78  | RF0   | 127  | ARG  | CD-NE-CZ    | 5.04  | 131.46      | 124.40   |
| 7   | L70   | 1    | A    | N9-C1'-C2'  | 5.04  | 117.55      | 112.00   |
| 2   | R60   | 1050 | G    | O4'-C1'-N9  | 5.04  | 112.03      | 108.50   |
| 2   | S60   | 1050 | G    | O4'-C1'-N9  | 5.04  | 112.03      | 108.50   |
| 1   | L50   | 179  | U    | N3-C2-O2    | -5.04 | 118.67      | 122.20   |
| 1   | K50   | 179  | U    | N3-C2-O2    | -5.04 | 118.67      | 122.20   |
| 1   | K50   | 2045 | C    | O5'-C5'-C4' | 5.04  | 113.43      | 109.40   |
| 1   | L50   | 2045 | C    | O5'-C5'-C4' | 5.04  | 113.43      | 109.40   |
| 2   | R60   | 236  | U    | N3-C4-O4    | 5.03  | 122.92      | 119.40   |
| 2   | S60   | 236  | U    | N3-C4-O4    | 5.03  | 122.92      | 119.40   |
| 1   | K50   | 368  | C    | N3-C4-C5    | 5.03  | 123.91      | 121.90   |
| 1   | L50   | 368  | C    | N3-C4-C5    | 5.03  | 123.91      | 121.90   |
| 2   | S60   | 1026 | U    | C6-N1-C1'   | 5.02  | 128.23      | 121.20   |
| 2   | R60   | 1026 | U    | C6-N1-C1'   | 5.02  | 128.23      | 121.20   |
| 2   | R60   | 820  | G    | C8-N9-C1'   | -5.01 | 120.49      | 127.00   |
| 2   | S60   | 820  | G    | C8-N9-C1'   | -5.01 | 120.49      | 127.00   |
| 1   | K50   | 366  | G    | C1'-O4'-C4' | -5.00 | 105.90      | 109.90   |
| 1   | L50   | 366  | G    | C1'-O4'-C4' | -5.00 | 105.90      | 109.90   |

There are no chirality outliers.

All (76) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 8   | A     | 571 | TYR  | Peptide |
| 8   | A     | 572 | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 8   | A     | 583 | LYS  | Peptide   |
| 8   | A     | 585 | ALA  | Peptide   |
| 8   | A     | 691 | VAL  | Peptide   |
| 8   | B     | 571 | TYR  | Peptide   |
| 8   | B     | 572 | LEU  | Peptide   |
| 8   | B     | 583 | LYS  | Peptide   |
| 8   | B     | 585 | ALA  | Peptide   |
| 8   | B     | 691 | VAL  | Peptide   |
| 1   | K50   | 178 | G    | Sidechain |
| 1   | K50   | 179 | U    | Sidechain |
| 1   | K50   | 190 | G    | Sidechain |
| 1   | K50   | 201 | A    | Sidechain |
| 1   | K50   | 202 | G    | Sidechain |
| 1   | K50   | 204 | C    | Sidechain |
| 1   | K50   | 310 | A    | Sidechain |
| 1   | K50   | 311 | C    | Sidechain |
| 1   | K50   | 366 | G    | Sidechain |
| 1   | K50   | 367 | A    | Sidechain |
| 1   | K50   | 368 | C    | Sidechain |
| 1   | K50   | 483 | A    | Sidechain |
| 1   | K50   | 546 | G    | Sidechain |
| 29  | KHH   | 108 | TYR  | Sidechain |
| 32  | KJ0   | 46  | LYS  | Peptide   |
| 48  | KZ0   | 148 | TYR  | Peptide   |
| 1   | L50   | 178 | G    | Sidechain |
| 1   | L50   | 179 | U    | Sidechain |
| 1   | L50   | 190 | G    | Sidechain |
| 1   | L50   | 201 | A    | Sidechain |
| 1   | L50   | 202 | G    | Sidechain |
| 1   | L50   | 204 | C    | Sidechain |
| 1   | L50   | 310 | A    | Sidechain |
| 1   | L50   | 311 | C    | Sidechain |
| 1   | L50   | 366 | G    | Sidechain |
| 1   | L50   | 367 | A    | Sidechain |
| 1   | L50   | 368 | C    | Sidechain |
| 1   | L50   | 483 | A    | Sidechain |
| 1   | L50   | 546 | G    | Sidechain |
| 29  | LHH   | 108 | TYR  | Sidechain |
| 32  | LJ0   | 46  | LYS  | Peptide   |
| 48  | LZ0   | 148 | TYR  | Peptide   |
| 73  | RDD   | 47  | ILE  | Peptide   |
| 73  | RDD   | 61  | PHE  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 75  | RG0   | 177 | LEU  | Peptide   |
| 54  | RGG   | 126 | GLY  | Peptide   |
| 56  | RJ0   | 88  | ASP  | Peptide   |
| 61  | RO0   | 50  | ARG  | Sidechain |
| 65  | RS0   | 103 | THR  | Peptide   |
| 65  | RS0   | 108 | GLY  | Peptide   |
| 65  | RS0   | 111 | ILE  | Peptide   |
| 65  | RS0   | 112 | GLU  | Peptide   |
| 66  | RT0   | 100 | SER  | Peptide   |
| 66  | RT0   | 81  | SER  | Peptide   |
| 67  | RU0   | 55  | ARG  | Peptide   |
| 67  | RU0   | 81  | TYR  | Peptide   |
| 68  | RV0   | 6   | ARG  | Peptide   |
| 68  | RV0   | 8   | CYS  | Peptide   |
| 70  | RY0   | 40  | THR  | Peptide   |
| 73  | SDD   | 47  | ILE  | Peptide   |
| 73  | SDD   | 61  | PHE  | Peptide   |
| 75  | SG0   | 177 | LEU  | Peptide   |
| 54  | SGG   | 126 | GLY  | Peptide   |
| 56  | SJ0   | 88  | ASP  | Peptide   |
| 61  | SO0   | 50  | ARG  | Sidechain |
| 65  | SS0   | 103 | THR  | Peptide   |
| 65  | SS0   | 108 | GLY  | Peptide   |
| 65  | SS0   | 111 | ILE  | Peptide   |
| 65  | SS0   | 112 | GLU  | Peptide   |
| 66  | ST0   | 100 | SER  | Peptide   |
| 66  | ST0   | 81  | SER  | Peptide   |
| 67  | SU0   | 55  | ARG  | Peptide   |
| 67  | SU0   | 81  | TYR  | Peptide   |
| 68  | SV0   | 6   | ARG  | Peptide   |
| 68  | SV0   | 8   | CYS  | Peptide   |
| 70  | SY0   | 40  | THR  | Peptide   |

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 3   | D     | 162/164 (99%)  | 145 (90%) | 17 (10%) | 0        | 100         | 100 |
| 3   | E     | 162/164 (99%)  | 145 (90%) | 17 (10%) | 0        | 100         | 100 |
| 4   | KGG   | 102/106 (96%)  | 97 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 4   | LGG   | 102/106 (96%)  | 97 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 5   | RB0   | 202/230 (88%)  | 197 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 5   | SB0   | 202/230 (88%)  | 197 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 6   | RC0   | 224/248 (90%)  | 203 (91%) | 21 (9%)  | 0        | 100         | 100 |
| 6   | SC0   | 224/248 (90%)  | 203 (91%) | 21 (9%)  | 0        | 100         | 100 |
| 8   | A     | 845/847 (100%) | 767 (91%) | 77 (9%)  | 1 (0%)   | 48          | 83  |
| 8   | B     | 845/847 (100%) | 767 (91%) | 77 (9%)  | 1 (0%)   | 48          | 83  |
| 9   | K     | 208/210 (99%)  | 199 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 9   | L     | 208/210 (99%)  | 199 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 10  | M     | 267/269 (99%)  | 254 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 10  | N     | 267/269 (99%)  | 254 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 11  | KMM   | 50/127 (39%)   | 36 (72%)  | 13 (26%) | 1 (2%)   | 6           | 31  |
| 11  | LMM   | 50/127 (39%)   | 36 (72%)  | 13 (26%) | 1 (2%)   | 6           | 31  |
| 12  | RBB   | 79/82 (96%)    | 76 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 12  | SBB   | 79/82 (96%)    | 76 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 13  | RAA   | 99/102 (97%)   | 93 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 13  | SAA   | 99/102 (97%)   | 93 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 14  | KOO   | 98/104 (94%)   | 91 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 14  | LOO   | 98/104 (94%)   | 91 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 15  | KPP   | 85/89 (96%)    | 79 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 15  | LPP   | 85/89 (96%)    | 79 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 16  | KJJ   | 87/92 (95%)    | 81 (93%)  | 6 (7%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 16  | LJJ   | 87/92 (95%)   | 80 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 17  | LA0   | 243/246 (99%) | 227 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 17  | LA02  | 243/246 (99%) | 227 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 18  | KAA   | 145/147 (99%) | 138 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 18  | LAA   | 145/147 (99%) | 138 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 19  | KB0   | 381/392 (97%) | 365 (96%) | 16 (4%)  | 0        | 100         | 100 |
| 19  | LB0   | 381/392 (97%) | 365 (96%) | 16 (4%)  | 0        | 100         | 100 |
| 20  | KC0   | 325/328 (99%) | 307 (94%) | 18 (6%)  | 0        | 100         | 100 |
| 20  | LC0   | 325/328 (99%) | 306 (94%) | 19 (6%)  | 0        | 100         | 100 |
| 21  | KCC   | 97/110 (88%)  | 95 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 21  | LCC   | 97/110 (88%)  | 95 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 22  | KDD   | 107/110 (97%) | 102 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 22  | LDD   | 107/110 (97%) | 102 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 23  | KE0   | 163/171 (95%) | 153 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 23  | LE0   | 163/171 (95%) | 153 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 24  | KEE   | 133/139 (96%) | 125 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 24  | LEE   | 133/139 (96%) | 125 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 25  | KF0   | 229/235 (97%) | 216 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 25  | LF0   | 229/235 (97%) | 216 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 26  | KFF   | 109/111 (98%) | 98 (90%)  | 11 (10%) | 0        | 100         | 100 |
| 26  | LFF   | 109/111 (98%) | 97 (89%)  | 12 (11%) | 0        | 100         | 100 |
| 27  | KG0   | 197/206 (96%) | 187 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 27  | LG0   | 197/206 (96%) | 187 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 28  | KH0   | 181/187 (97%) | 168 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 28  | LH0   | 181/187 (97%) | 168 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 29  | KHH   | 117/119 (98%) | 111 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 29  | LHH   | 117/119 (98%) | 111 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 30  | KI0   | 215/218 (99%) | 205 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 30  | LI0   | 215/218 (99%) | 205 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 31  | KII   | 95/98 (97%)   | 92 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 31  | LII   | 95/98 (97%)   | 92 (97%)  | 3 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 32  | KJ0   | 165/171 (96%) | 143 (87%) | 21 (13%) | 1 (1%)   | 21          | 59  |
| 32  | LJ0   | 165/171 (96%) | 143 (87%) | 21 (13%) | 1 (1%)   | 21          | 59  |
| 33  | KL0   | 162/165 (98%) | 151 (93%) | 9 (6%)   | 2 (1%)   | 10          | 44  |
| 33  | LL0   | 162/165 (98%) | 151 (93%) | 9 (6%)   | 2 (1%)   | 10          | 44  |
| 34  | KLL   | 49/52 (94%)   | 47 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 34  | LLL   | 49/52 (94%)   | 47 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 35  | KM0   | 113/122 (93%) | 96 (85%)  | 17 (15%) | 0        | 100         | 100 |
| 35  | LM0   | 113/122 (93%) | 95 (84%)  | 18 (16%) | 0        | 100         | 100 |
| 36  | KN0   | 201/204 (98%) | 189 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 36  | LN0   | 201/204 (98%) | 189 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 37  | KO0   | 196/198 (99%) | 191 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 37  | LO0   | 196/198 (99%) | 191 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 38  | KP0   | 152/167 (91%) | 143 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 38  | LP0   | 152/167 (91%) | 143 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 39  | KQ0   | 180/183 (98%) | 169 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 39  | LQ0   | 180/183 (98%) | 168 (93%) | 12 (7%)  | 0        | 100         | 100 |
| 40  | KR0   | 162/168 (96%) | 155 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 40  | LR0   | 162/168 (96%) | 155 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 41  | KS0   | 168/171 (98%) | 157 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 41  | LS0   | 168/171 (98%) | 158 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 42  | KT0   | 154/158 (98%) | 141 (92%) | 13 (8%)  | 0        | 100         | 100 |
| 42  | LT0   | 154/158 (98%) | 141 (92%) | 13 (8%)  | 0        | 100         | 100 |
| 43  | KU0   | 98/113 (87%)  | 93 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 43  | LU0   | 98/113 (87%)  | 93 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 44  | KV0   | 139/142 (98%) | 131 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 44  | LV0   | 139/142 (98%) | 131 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 45  | KW0   | 100/131 (76%) | 93 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 45  | LW0   | 100/131 (76%) | 93 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 46  | KX0   | 110/113 (97%) | 107 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 46  | LX0   | 110/113 (97%) | 106 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 47  | KY0   | 129/131 (98%) | 119 (92%) | 10 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 47  | LY0   | 129/131 (98%) | 119 (92%)  | 10 (8%)  | 0        | 100         | 100 |
| 48  | KZ0   | 116/153 (76%) | 110 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 48  | LZ0   | 116/153 (76%) | 110 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 49  | MD1   | 149/151 (99%) | 124 (83%)  | 22 (15%) | 3 (2%)   | 6           | 31  |
| 49  | ND1   | 149/151 (99%) | 124 (83%)  | 22 (15%) | 3 (2%)   | 6           | 31  |
| 50  | RA0   | 218/233 (94%) | 201 (92%)  | 17 (8%)  | 0        | 100         | 100 |
| 50  | SA0   | 218/233 (94%) | 201 (92%)  | 17 (8%)  | 0        | 100         | 100 |
| 51  | RCC   | 60/65 (92%)   | 60 (100%)  | 0        | 0        | 100         | 100 |
| 51  | SCC   | 60/65 (92%)   | 60 (100%)  | 0        | 0        | 100         | 100 |
| 52  | RE0   | 258/280 (92%) | 233 (90%)  | 25 (10%) | 0        | 100         | 100 |
| 52  | SE0   | 258/280 (92%) | 233 (90%)  | 25 (10%) | 0        | 100         | 100 |
| 53  | REE   | 54/60 (90%)   | 51 (94%)   | 3 (6%)   | 0        | 100         | 100 |
| 53  | SEE   | 54/60 (90%)   | 51 (94%)   | 3 (6%)   | 0        | 100         | 100 |
| 54  | RGG   | 315/326 (97%) | 285 (90%)  | 30 (10%) | 0        | 100         | 100 |
| 54  | SGG   | 315/326 (97%) | 285 (90%)  | 30 (10%) | 0        | 100         | 100 |
| 55  | RI0   | 165/173 (95%) | 157 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 55  | SI0   | 165/173 (95%) | 157 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 56  | RJ0   | 166/184 (90%) | 150 (90%)  | 16 (10%) | 0        | 100         | 100 |
| 56  | SJ0   | 166/184 (90%) | 150 (90%)  | 16 (10%) | 0        | 100         | 100 |
| 57  | RK0   | 86/107 (80%)  | 74 (86%)   | 12 (14%) | 0        | 100         | 100 |
| 57  | SK0   | 86/107 (80%)  | 74 (86%)   | 12 (14%) | 0        | 100         | 100 |
| 58  | RL0   | 148/155 (96%) | 143 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 58  | SL0   | 148/155 (96%) | 144 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 59  | RM0   | 109/130 (84%) | 109 (100%) | 0        | 0        | 100         | 100 |
| 59  | SM0   | 109/130 (84%) | 109 (100%) | 0        | 0        | 100         | 100 |
| 60  | RN0   | 140/143 (98%) | 132 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 60  | SN0   | 140/143 (98%) | 132 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 61  | RO0   | 127/135 (94%) | 126 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 61  | SO0   | 127/135 (94%) | 126 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 62  | RP0   | 115/163 (71%) | 105 (91%)  | 10 (9%)  | 0        | 100         | 100 |
| 62  | SP0   | 115/163 (71%) | 105 (91%)  | 10 (9%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 63  | RQ0   | 140/143 (98%) | 135 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 63  | SQ0   | 140/143 (98%) | 135 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 64  | RR0   | 117/120 (98%) | 95 (81%)  | 22 (19%) | 0        | 100         | 100 |
| 64  | SR0   | 117/120 (98%) | 95 (81%)  | 22 (19%) | 0        | 100         | 100 |
| 65  | RS0   | 142/160 (89%) | 121 (85%) | 21 (15%) | 0        | 100         | 100 |
| 65  | SS0   | 142/160 (89%) | 121 (85%) | 21 (15%) | 0        | 100         | 100 |
| 66  | RT0   | 140/143 (98%) | 125 (89%) | 15 (11%) | 0        | 100         | 100 |
| 66  | ST0   | 140/143 (98%) | 125 (89%) | 15 (11%) | 0        | 100         | 100 |
| 67  | RU0   | 98/119 (82%)  | 89 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 67  | SU0   | 98/119 (82%)  | 89 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 68  | RV0   | 63/67 (94%)   | 51 (81%)  | 12 (19%) | 0        | 100         | 100 |
| 68  | SV0   | 63/67 (94%)   | 51 (81%)  | 12 (19%) | 0        | 100         | 100 |
| 69  | RX0   | 138/141 (98%) | 117 (85%) | 21 (15%) | 0        | 100         | 100 |
| 69  | SX0   | 138/141 (98%) | 117 (85%) | 21 (15%) | 0        | 100         | 100 |
| 70  | RY0   | 134/146 (92%) | 118 (88%) | 16 (12%) | 0        | 100         | 100 |
| 70  | SY0   | 134/146 (92%) | 119 (89%) | 15 (11%) | 0        | 100         | 100 |
| 71  | RZ0   | 74/128 (58%)  | 66 (89%)  | 8 (11%)  | 0        | 100         | 100 |
| 71  | SZ0   | 74/128 (58%)  | 66 (89%)  | 8 (11%)  | 0        | 100         | 100 |
| 72  | KD0   | 279/291 (96%) | 269 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 72  | LD0   | 279/291 (96%) | 268 (96%) | 11 (4%)  | 0        | 100         | 100 |
| 73  | RDD   | 63/65 (97%)   | 50 (79%)  | 13 (21%) | 0        | 100         | 100 |
| 73  | SDD   | 63/65 (97%)   | 50 (79%)  | 13 (21%) | 0        | 100         | 100 |
| 74  | RD0   | 214/242 (88%) | 208 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 74  | SD0   | 214/242 (88%) | 207 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 75  | RG0   | 227/230 (99%) | 209 (92%) | 17 (8%)  | 1 (0%)   | 30          | 67  |
| 75  | SG0   | 227/230 (99%) | 209 (92%) | 17 (8%)  | 1 (0%)   | 30          | 67  |
| 76  | RH0   | 161/164 (98%) | 152 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 76  | SH0   | 161/164 (98%) | 152 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 77  | RW0   | 126/128 (98%) | 117 (93%) | 8 (6%)   | 1 (1%)   | 16          | 54  |
| 77  | SW0   | 126/128 (98%) | 117 (93%) | 8 (6%)   | 1 (1%)   | 16          | 54  |
| 78  | RF0   | 190/195 (97%) | 173 (91%) | 17 (9%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 78  | SF0   | 190/195 (97%)     | 173 (91%)   | 17 (9%)   | 0        | 100         | 100 |
| 79  | RFF   | 52/150 (35%)      | 48 (92%)    | 4 (8%)    | 0        | 100         | 100 |
| 79  | SFF   | 52/150 (35%)      | 48 (92%)    | 4 (8%)    | 0        | 100         | 100 |
| All | All   | 24214/25932 (93%) | 22465 (93%) | 1729 (7%) | 20 (0%)  | 49          | 83  |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | KL0   | 44  | TYR  |
| 75  | RG0   | 173 | ASP  |
| 33  | LL0   | 44  | TYR  |
| 75  | SG0   | 173 | ASP  |
| 11  | KMM   | 108 | ALA  |
| 33  | KL0   | 142 | MET  |
| 49  | ND1   | 37  | LYS  |
| 11  | LMM   | 108 | ALA  |
| 33  | LL0   | 142 | MET  |
| 49  | MD1   | 37  | LYS  |
| 49  | ND1   | 30  | SER  |
| 49  | ND1   | 69  | MET  |
| 49  | MD1   | 30  | SER  |
| 49  | MD1   | 69  | MET  |
| 77  | RW0   | 56  | GLU  |
| 77  | SW0   | 56  | GLU  |
| 8   | B     | 29  | LYS  |
| 8   | A     | 29  | LYS  |
| 32  | KJ0   | 141 | VAL  |
| 32  | LJ0   | 141 | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | D     | 137/137 (100%) | 137 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | E     | 137/137 (100%) | 137 (100%) | 0        | 100         | 100 |
| 4   | KGG   | 88/90 (98%)    | 87 (99%)   | 1 (1%)   | 65          | 76  |
| 4   | LGG   | 88/90 (98%)    | 87 (99%)   | 1 (1%)   | 65          | 76  |
| 5   | RB0   | 182/203 (90%)  | 181 (100%) | 1 (0%)   | 81          | 83  |
| 5   | SB0   | 182/203 (90%)  | 181 (100%) | 1 (0%)   | 81          | 83  |
| 6   | RC0   | 188/209 (90%)  | 188 (100%) | 0        | 100         | 100 |
| 6   | SC0   | 188/209 (90%)  | 188 (100%) | 0        | 100         | 100 |
| 8   | A     | 732/732 (100%) | 732 (100%) | 0        | 100         | 100 |
| 8   | B     | 732/732 (100%) | 732 (100%) | 0        | 100         | 100 |
| 9   | K     | 194/194 (100%) | 194 (100%) | 0        | 100         | 100 |
| 9   | L     | 194/194 (100%) | 194 (100%) | 0        | 100         | 100 |
| 10  | M     | 241/241 (100%) | 241 (100%) | 0        | 100         | 100 |
| 10  | N     | 241/241 (100%) | 241 (100%) | 0        | 100         | 100 |
| 11  | KMM   | 46/112 (41%)   | 42 (91%)   | 4 (9%)   | 9           | 29  |
| 11  | LMM   | 46/112 (41%)   | 42 (91%)   | 4 (9%)   | 9           | 29  |
| 12  | RBB   | 72/73 (99%)    | 71 (99%)   | 1 (1%)   | 59          | 72  |
| 12  | SBB   | 72/73 (99%)    | 71 (99%)   | 1 (1%)   | 59          | 72  |
| 13  | RAA   | 92/93 (99%)    | 92 (100%)  | 0        | 100         | 100 |
| 13  | SAA   | 92/93 (99%)    | 92 (100%)  | 0        | 100         | 100 |
| 14  | KOO   | 85/89 (96%)    | 85 (100%)  | 0        | 100         | 100 |
| 14  | LOO   | 85/89 (96%)    | 85 (100%)  | 0        | 100         | 100 |
| 15  | KPP   | 75/77 (97%)    | 75 (100%)  | 0        | 100         | 100 |
| 15  | LPP   | 75/77 (97%)    | 75 (100%)  | 0        | 100         | 100 |
| 16  | KJJ   | 78/81 (96%)    | 78 (100%)  | 0        | 100         | 100 |
| 16  | LJJ   | 78/81 (96%)    | 78 (100%)  | 0        | 100         | 100 |
| 17  | LA0   | 202/203 (100%) | 200 (99%)  | 2 (1%)   | 68          | 78  |
| 17  | LA02  | 202/203 (100%) | 200 (99%)  | 2 (1%)   | 68          | 78  |
| 18  | KAA   | 123/123 (100%) | 121 (98%)  | 2 (2%)   | 55          | 70  |
| 18  | LAA   | 123/123 (100%) | 121 (98%)  | 2 (2%)   | 55          | 70  |
| 19  | KB0   | 328/336 (98%)  | 328 (100%) | 0        | 100         | 100 |
| 19  | LB0   | 328/336 (98%)  | 328 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 20  | KC0   | 277/278 (100%) | 277 (100%) | 0        | 100         | 100 |
| 20  | LC0   | 277/278 (100%) | 277 (100%) | 0        | 100         | 100 |
| 21  | KCC   | 87/97 (90%)    | 87 (100%)  | 0        | 100         | 100 |
| 21  | LCC   | 87/97 (90%)    | 87 (100%)  | 0        | 100         | 100 |
| 22  | KDD   | 99/100 (99%)   | 99 (100%)  | 0        | 100         | 100 |
| 22  | LDD   | 99/100 (99%)   | 99 (100%)  | 0        | 100         | 100 |
| 23  | KE0   | 153/159 (96%)  | 153 (100%) | 0        | 100         | 100 |
| 23  | LE0   | 153/159 (96%)  | 153 (100%) | 0        | 100         | 100 |
| 24  | KEE   | 118/122 (97%)  | 118 (100%) | 0        | 100         | 100 |
| 24  | LEE   | 118/122 (97%)  | 118 (100%) | 0        | 100         | 100 |
| 25  | KF0   | 212/216 (98%)  | 212 (100%) | 0        | 100         | 100 |
| 25  | LF0   | 212/216 (98%)  | 212 (100%) | 0        | 100         | 100 |
| 26  | KFF   | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 26  | LFF   | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 27  | KG0   | 183/190 (96%)  | 182 (100%) | 1 (0%)   | 81          | 83  |
| 27  | LG0   | 183/190 (96%)  | 182 (100%) | 1 (0%)   | 81          | 83  |
| 28  | KH0   | 165/169 (98%)  | 164 (99%)  | 1 (1%)   | 78          | 83  |
| 28  | LH0   | 165/169 (98%)  | 164 (99%)  | 1 (1%)   | 78          | 83  |
| 29  | KHH   | 110/110 (100%) | 109 (99%)  | 1 (1%)   | 70          | 79  |
| 29  | LHH   | 110/110 (100%) | 109 (99%)  | 1 (1%)   | 70          | 79  |
| 30  | KI0   | 188/189 (100%) | 188 (100%) | 0        | 100         | 100 |
| 30  | LI0   | 188/189 (100%) | 188 (100%) | 0        | 100         | 100 |
| 31  | KII   | 84/84 (100%)   | 83 (99%)   | 1 (1%)   | 63          | 75  |
| 31  | LII   | 84/84 (100%)   | 83 (99%)   | 1 (1%)   | 63          | 75  |
| 32  | KJ0   | 146/149 (98%)  | 146 (100%) | 0        | 100         | 100 |
| 32  | LJ0   | 146/149 (98%)  | 146 (100%) | 0        | 100         | 100 |
| 33  | KL0   | 148/149 (99%)  | 144 (97%)  | 4 (3%)   | 39          | 61  |
| 33  | LL0   | 148/149 (99%)  | 144 (97%)  | 4 (3%)   | 39          | 61  |
| 34  | KLL   | 46/47 (98%)    | 46 (100%)  | 0        | 100         | 100 |
| 34  | LLL   | 46/47 (98%)    | 46 (100%)  | 0        | 100         | 100 |
| 35  | KM0   | 110/117 (94%)  | 109 (99%)  | 1 (1%)   | 70          | 79  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 35  | LM0   | 110/117 (94%)  | 109 (99%)  | 1 (1%)   | 70          | 79  |
| 36  | KN0   | 175/176 (99%)  | 175 (100%) | 0        | 100         | 100 |
| 36  | LN0   | 175/176 (99%)  | 175 (100%) | 0        | 100         | 100 |
| 37  | KO0   | 178/178 (100%) | 177 (99%)  | 1 (1%)   | 78          | 83  |
| 37  | LO0   | 178/178 (100%) | 177 (99%)  | 1 (1%)   | 78          | 83  |
| 38  | KP0   | 135/147 (92%)  | 135 (100%) | 0        | 100         | 100 |
| 38  | LP0   | 135/147 (92%)  | 135 (100%) | 0        | 100         | 100 |
| 39  | KQ0   | 165/166 (99%)  | 165 (100%) | 0        | 100         | 100 |
| 39  | LQ0   | 165/166 (99%)  | 165 (100%) | 0        | 100         | 100 |
| 40  | KR0   | 142/145 (98%)  | 142 (100%) | 0        | 100         | 100 |
| 40  | LR0   | 142/145 (98%)  | 142 (100%) | 0        | 100         | 100 |
| 41  | KS0   | 155/156 (99%)  | 153 (99%)  | 2 (1%)   | 61          | 74  |
| 41  | LS0   | 155/156 (99%)  | 153 (99%)  | 2 (1%)   | 61          | 74  |
| 42  | KT0   | 140/142 (99%)  | 139 (99%)  | 1 (1%)   | 76          | 81  |
| 42  | LT0   | 140/142 (99%)  | 139 (99%)  | 1 (1%)   | 76          | 81  |
| 43  | KU0   | 89/98 (91%)    | 88 (99%)   | 1 (1%)   | 65          | 76  |
| 43  | LU0   | 89/98 (91%)    | 88 (99%)   | 1 (1%)   | 65          | 76  |
| 44  | KV0   | 113/114 (99%)  | 113 (100%) | 0        | 100         | 100 |
| 44  | LV0   | 113/114 (99%)  | 113 (100%) | 0        | 100         | 100 |
| 45  | KW0   | 93/120 (78%)   | 93 (100%)  | 0        | 100         | 100 |
| 45  | LW0   | 93/120 (78%)   | 93 (100%)  | 0        | 100         | 100 |
| 46  | KX0   | 92/93 (99%)    | 92 (100%)  | 0        | 100         | 100 |
| 46  | LX0   | 92/93 (99%)    | 92 (100%)  | 0        | 100         | 100 |
| 47  | KY0   | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 47  | LY0   | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 48  | KZ0   | 106/141 (75%)  | 106 (100%) | 0        | 100         | 100 |
| 48  | LZ0   | 106/141 (75%)  | 106 (100%) | 0        | 100         | 100 |
| 49  | MD1   | 139/139 (100%) | 136 (98%)  | 3 (2%)   | 45          | 64  |
| 49  | ND1   | 139/139 (100%) | 136 (98%)  | 3 (2%)   | 45          | 64  |
| 50  | RA0   | 194/206 (94%)  | 194 (100%) | 0        | 100         | 100 |
| 50  | SA0   | 194/206 (94%)  | 194 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 51  | RCC   | 51/54 (94%)   | 50 (98%)   | 1 (2%)   | 48          | 66  |
| 51  | SCC   | 51/54 (94%)   | 50 (98%)   | 1 (2%)   | 48          | 66  |
| 52  | RE0   | 231/251 (92%) | 231 (100%) | 0        | 100         | 100 |
| 52  | SE0   | 231/251 (92%) | 231 (100%) | 0        | 100         | 100 |
| 53  | REE   | 44/47 (94%)   | 44 (100%)  | 0        | 100         | 100 |
| 53  | SEE   | 44/47 (94%)   | 44 (100%)  | 0        | 100         | 100 |
| 54  | RGG   | 282/288 (98%) | 282 (100%) | 0        | 100         | 100 |
| 54  | SGG   | 282/288 (98%) | 282 (100%) | 0        | 100         | 100 |
| 55  | RI0   | 147/153 (96%) | 147 (100%) | 0        | 100         | 100 |
| 55  | SI0   | 147/153 (96%) | 147 (100%) | 0        | 100         | 100 |
| 56  | RJ0   | 152/165 (92%) | 152 (100%) | 0        | 100         | 100 |
| 56  | SJ0   | 152/165 (92%) | 152 (100%) | 0        | 100         | 100 |
| 57  | RK0   | 83/99 (84%)   | 83 (100%)  | 0        | 100         | 100 |
| 57  | SK0   | 83/99 (84%)   | 83 (100%)  | 0        | 100         | 100 |
| 58  | RL0   | 140/145 (97%) | 139 (99%)  | 1 (1%)   | 76          | 81  |
| 58  | SL0   | 140/145 (97%) | 139 (99%)  | 1 (1%)   | 76          | 81  |
| 59  | RM0   | 99/114 (87%)  | 99 (100%)  | 0        | 100         | 100 |
| 59  | SM0   | 99/114 (87%)  | 99 (100%)  | 0        | 100         | 100 |
| 60  | RN0   | 126/127 (99%) | 126 (100%) | 0        | 100         | 100 |
| 60  | SN0   | 126/127 (99%) | 126 (100%) | 0        | 100         | 100 |
| 61  | RO0   | 102/108 (94%) | 102 (100%) | 0        | 100         | 100 |
| 61  | SO0   | 102/108 (94%) | 102 (100%) | 0        | 100         | 100 |
| 62  | RP0   | 107/144 (74%) | 106 (99%)  | 1 (1%)   | 70          | 79  |
| 62  | SP0   | 107/144 (74%) | 106 (99%)  | 1 (1%)   | 70          | 79  |
| 63  | RQ0   | 120/121 (99%) | 120 (100%) | 0        | 100         | 100 |
| 63  | SQ0   | 120/121 (99%) | 120 (100%) | 0        | 100         | 100 |
| 64  | RR0   | 109/111 (98%) | 109 (100%) | 0        | 100         | 100 |
| 64  | SR0   | 109/111 (98%) | 109 (100%) | 0        | 100         | 100 |
| 65  | RS0   | 125/138 (91%) | 125 (100%) | 0        | 100         | 100 |
| 65  | SS0   | 125/138 (91%) | 125 (100%) | 0        | 100         | 100 |
| 66  | RT0   | 129/130 (99%) | 129 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 66  | ST0   | 129/130 (99%)     | 129 (100%)   | 0        | 100         | 100 |
| 67  | RU0   | 92/110 (84%)      | 91 (99%)     | 1 (1%)   | 65          | 76  |
| 67  | SU0   | 92/110 (84%)      | 91 (99%)     | 1 (1%)   | 65          | 76  |
| 68  | RV0   | 61/63 (97%)       | 61 (100%)    | 0        | 100         | 100 |
| 68  | SV0   | 61/63 (97%)       | 61 (100%)    | 0        | 100         | 100 |
| 69  | RX0   | 115/116 (99%)     | 114 (99%)    | 1 (1%)   | 70          | 79  |
| 69  | SX0   | 115/116 (99%)     | 114 (99%)    | 1 (1%)   | 70          | 79  |
| 70  | RY0   | 126/136 (93%)     | 124 (98%)    | 2 (2%)   | 55          | 70  |
| 70  | SY0   | 126/136 (93%)     | 124 (98%)    | 2 (2%)   | 55          | 70  |
| 71  | RZ0   | 73/118 (62%)      | 73 (100%)    | 0        | 100         | 100 |
| 71  | SZ0   | 73/118 (62%)      | 73 (100%)    | 0        | 100         | 100 |
| 72  | KD0   | 251/261 (96%)     | 251 (100%)   | 0        | 100         | 100 |
| 72  | LD0   | 251/261 (96%)     | 251 (100%)   | 0        | 100         | 100 |
| 73  | RDD   | 57/57 (100%)      | 57 (100%)    | 0        | 100         | 100 |
| 73  | SDD   | 57/57 (100%)      | 57 (100%)    | 0        | 100         | 100 |
| 74  | RD0   | 189/215 (88%)     | 189 (100%)   | 0        | 100         | 100 |
| 74  | SD0   | 189/215 (88%)     | 189 (100%)   | 0        | 100         | 100 |
| 75  | RG0   | 199/200 (100%)    | 198 (100%)   | 1 (0%)   | 81          | 83  |
| 75  | SG0   | 199/200 (100%)    | 198 (100%)   | 1 (0%)   | 81          | 83  |
| 76  | RH0   | 153/154 (99%)     | 153 (100%)   | 0        | 100         | 100 |
| 76  | SH0   | 153/154 (99%)     | 153 (100%)   | 0        | 100         | 100 |
| 77  | RW0   | 111/111 (100%)    | 111 (100%)   | 0        | 100         | 100 |
| 77  | SW0   | 111/111 (100%)    | 111 (100%)   | 0        | 100         | 100 |
| 78  | RF0   | 167/170 (98%)     | 166 (99%)    | 1 (1%)   | 78          | 83  |
| 78  | SF0   | 167/170 (98%)     | 166 (99%)    | 1 (1%)   | 78          | 83  |
| 79  | RFF   | 48/136 (35%)      | 48 (100%)    | 0        | 100         | 100 |
| 79  | SFF   | 48/136 (35%)      | 48 (100%)    | 0        | 100         | 100 |
| All | All   | 21616/22892 (94%) | 21542 (100%) | 74 (0%)  | 84          | 86  |

All (74) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | KGG   | 71  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | RB0   | 228 | ARG  |
| 11  | KMM   | 91  | ARG  |
| 11  | KMM   | 92  | LYS  |
| 11  | KMM   | 103 | HIS  |
| 11  | KMM   | 105 | ARG  |
| 12  | RBB   | 64  | ARG  |
| 17  | LA0   | 64  | LYS  |
| 17  | LA0   | 148 | ARG  |
| 18  | KAA   | 49  | HIS  |
| 18  | KAA   | 54  | ARG  |
| 27  | KG0   | 72  | ARG  |
| 28  | KH0   | 94  | LYS  |
| 29  | KHH   | 105 | THR  |
| 31  | KII   | 72  | LYS  |
| 33  | KL0   | 1   | MET  |
| 33  | KL0   | 2   | ARG  |
| 33  | KL0   | 12  | PHE  |
| 33  | KL0   | 97  | ARG  |
| 35  | KM0   | 76  | LYS  |
| 37  | KO0   | 169 | LYS  |
| 41  | KS0   | 95  | ARG  |
| 41  | KS0   | 157 | ARG  |
| 42  | KT0   | 55  | LYS  |
| 43  | KU0   | 68  | LYS  |
| 49  | ND1   | 2   | LYS  |
| 49  | ND1   | 32  | CYS  |
| 49  | ND1   | 68  | GLN  |
| 51  | RCC   | 62  | ARG  |
| 58  | RL0   | 67  | LYS  |
| 62  | RP0   | 135 | ARG  |
| 67  | RU0   | 55  | ARG  |
| 69  | RX0   | 51  | LYS  |
| 70  | RY0   | 134 | LYS  |
| 70  | RY0   | 136 | ARG  |
| 75  | RG0   | 92  | ARG  |
| 78  | RF0   | 126 | LYS  |
| 4   | LGG   | 71  | LYS  |
| 5   | SB0   | 228 | ARG  |
| 11  | LMM   | 91  | ARG  |
| 11  | LMM   | 92  | LYS  |
| 11  | LMM   | 103 | HIS  |
| 11  | LMM   | 105 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | SBB   | 64  | ARG  |
| 17  | LA02  | 64  | LYS  |
| 17  | LA02  | 148 | ARG  |
| 18  | LAA   | 49  | HIS  |
| 18  | LAA   | 54  | ARG  |
| 27  | LG0   | 72  | ARG  |
| 28  | LH0   | 94  | LYS  |
| 29  | LHH   | 105 | THR  |
| 31  | LII   | 72  | LYS  |
| 33  | LL0   | 1   | MET  |
| 33  | LL0   | 2   | ARG  |
| 33  | LL0   | 12  | PHE  |
| 33  | LL0   | 97  | ARG  |
| 35  | LM0   | 76  | LYS  |
| 37  | LO0   | 169 | LYS  |
| 41  | LS0   | 95  | ARG  |
| 41  | LS0   | 157 | ARG  |
| 42  | LT0   | 55  | LYS  |
| 43  | LU0   | 68  | LYS  |
| 49  | MD1   | 2   | LYS  |
| 49  | MD1   | 32  | CYS  |
| 49  | MD1   | 68  | GLN  |
| 51  | SCC   | 62  | ARG  |
| 58  | SL0   | 67  | LYS  |
| 62  | SP0   | 135 | ARG  |
| 67  | SU0   | 55  | ARG  |
| 69  | SX0   | 51  | LYS  |
| 70  | SY0   | 134 | LYS  |
| 70  | SY0   | 136 | ARG  |
| 75  | SG0   | 92  | ARG  |
| 78  | SF0   | 126 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 165 | HIS  |
| 8   | B     | 460 | ASN  |
| 8   | B     | 651 | ASN  |
| 8   | B     | 809 | GLN  |
| 9   | K     | 30  | GLN  |
| 9   | K     | 53  | GLN  |
| 9   | K     | 139 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | K     | 164 | HIS  |
| 8   | A     | 165 | HIS  |
| 8   | A     | 460 | ASN  |
| 8   | A     | 651 | ASN  |
| 8   | A     | 809 | GLN  |
| 9   | L     | 30  | GLN  |
| 9   | L     | 53  | GLN  |
| 9   | L     | 139 | ASN  |
| 9   | L     | 164 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | K50   | 2603/2618 (99%) | 755 (29%)         | 56 (2%)         |
| 1   | L50   | 2603/2618 (99%) | 755 (29%)         | 56 (2%)         |
| 2   | R60   | 1353/1368 (98%) | 561 (41%)         | 54 (3%)         |
| 2   | S60   | 1353/1368 (98%) | 561 (41%)         | 54 (3%)         |
| 7   | K70   | 118/119 (99%)   | 29 (24%)          | 2 (1%)          |
| 7   | L70   | 118/119 (99%)   | 29 (24%)          | 2 (1%)          |
| All | All   | 8148/8210 (99%) | 2690 (33%)        | 224 (2%)        |

All (2690) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 2   | U    |
| 1   | K50   | 3   | A    |
| 1   | K50   | 14  | G    |
| 1   | K50   | 15  | G    |
| 1   | K50   | 16  | G    |
| 1   | K50   | 17  | A    |
| 1   | K50   | 22  | U    |
| 1   | K50   | 23  | U    |
| 1   | K50   | 24  | G    |
| 1   | K50   | 43  | G    |
| 1   | K50   | 47  | C    |
| 1   | K50   | 48  | A    |
| 1   | K50   | 49  | G    |
| 1   | K50   | 50  | C    |
| 1   | K50   | 52  | G    |
| 1   | K50   | 59  | A    |
| 1   | K50   | 61  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 62  | U    |
| 1   | K50   | 68  | G    |
| 1   | K50   | 70  | A    |
| 1   | K50   | 71  | G    |
| 1   | K50   | 73  | A    |
| 1   | K50   | 75  | C    |
| 1   | K50   | 76  | A    |
| 1   | K50   | 87  | C    |
| 1   | K50   | 88  | A    |
| 1   | K50   | 97  | A    |
| 1   | K50   | 99  | U    |
| 1   | K50   | 100 | A    |
| 1   | K50   | 110 | G    |
| 1   | K50   | 111 | C    |
| 1   | K50   | 112 | U    |
| 1   | K50   | 114 | G    |
| 1   | K50   | 118 | A    |
| 1   | K50   | 123 | U    |
| 1   | K50   | 124 | U    |
| 1   | K50   | 132 | A    |
| 1   | K50   | 134 | C    |
| 1   | K50   | 135 | A    |
| 1   | K50   | 139 | G    |
| 1   | K50   | 149 | A    |
| 1   | K50   | 151 | G    |
| 1   | K50   | 152 | A    |
| 1   | K50   | 156 | G    |
| 1   | K50   | 157 | A    |
| 1   | K50   | 158 | A    |
| 1   | K50   | 159 | A    |
| 1   | K50   | 160 | C    |
| 1   | K50   | 161 | U    |
| 1   | K50   | 163 | A    |
| 1   | K50   | 164 | C    |
| 1   | K50   | 166 | A    |
| 1   | K50   | 167 | G    |
| 1   | K50   | 168 | G    |
| 1   | K50   | 169 | A    |
| 1   | K50   | 171 | U    |
| 1   | K50   | 178 | G    |
| 1   | K50   | 179 | U    |
| 1   | K50   | 180 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 184 | G    |
| 1   | K50   | 191 | A    |
| 1   | K50   | 193 | C    |
| 1   | K50   | 194 | A    |
| 1   | K50   | 199 | A    |
| 1   | K50   | 200 | C    |
| 1   | K50   | 202 | G    |
| 1   | K50   | 209 | A    |
| 1   | K50   | 210 | G    |
| 1   | K50   | 213 | U    |
| 1   | K50   | 216 | U    |
| 1   | K50   | 224 | U    |
| 1   | K50   | 225 | G    |
| 1   | K50   | 226 | A    |
| 1   | K50   | 237 | A    |
| 1   | K50   | 240 | G    |
| 1   | K50   | 243 | A    |
| 1   | K50   | 251 | U    |
| 1   | K50   | 255 | U    |
| 1   | K50   | 256 | C    |
| 1   | K50   | 266 | A    |
| 1   | K50   | 268 | C    |
| 1   | K50   | 276 | U    |
| 1   | K50   | 284 | G    |
| 1   | K50   | 285 | A    |
| 1   | K50   | 287 | A    |
| 1   | K50   | 290 | C    |
| 1   | K50   | 298 | G    |
| 1   | K50   | 302 | U    |
| 1   | K50   | 308 | A    |
| 1   | K50   | 309 | U    |
| 1   | K50   | 310 | A    |
| 1   | K50   | 311 | C    |
| 1   | K50   | 312 | G    |
| 1   | K50   | 314 | U    |
| 1   | K50   | 315 | G    |
| 1   | K50   | 316 | A    |
| 1   | K50   | 318 | U    |
| 1   | K50   | 331 | U    |
| 1   | K50   | 332 | A    |
| 1   | K50   | 333 | A    |
| 1   | K50   | 340 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 343 | A    |
| 1   | K50   | 345 | G    |
| 1   | K50   | 346 | A    |
| 1   | K50   | 347 | G    |
| 1   | K50   | 352 | C    |
| 1   | K50   | 353 | A    |
| 1   | K50   | 358 | G    |
| 1   | K50   | 360 | A    |
| 1   | K50   | 361 | U    |
| 1   | K50   | 364 | A    |
| 1   | K50   | 366 | G    |
| 1   | K50   | 371 | A    |
| 1   | K50   | 384 | A    |
| 1   | K50   | 385 | C    |
| 1   | K50   | 392 | C    |
| 1   | K50   | 396 | G    |
| 1   | K50   | 398 | A    |
| 1   | K50   | 400 | U    |
| 1   | K50   | 405 | U    |
| 1   | K50   | 408 | C    |
| 1   | K50   | 416 | A    |
| 1   | K50   | 437 | G    |
| 1   | K50   | 444 | A    |
| 1   | K50   | 449 | U    |
| 1   | K50   | 454 | C    |
| 1   | K50   | 459 | C    |
| 1   | K50   | 467 | A    |
| 1   | K50   | 481 | G    |
| 1   | K50   | 488 | C    |
| 1   | K50   | 492 | G    |
| 1   | K50   | 494 | A    |
| 1   | K50   | 495 | A    |
| 1   | K50   | 498 | U    |
| 1   | K50   | 499 | G    |
| 1   | K50   | 501 | G    |
| 1   | K50   | 503 | A    |
| 1   | K50   | 504 | G    |
| 1   | K50   | 507 | G    |
| 1   | K50   | 508 | A    |
| 1   | K50   | 509 | A    |
| 1   | K50   | 510 | G    |
| 1   | K50   | 515 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 517 | A    |
| 1   | K50   | 523 | A    |
| 1   | K50   | 524 | G    |
| 1   | K50   | 526 | G    |
| 1   | K50   | 534 | A    |
| 1   | K50   | 535 | A    |
| 1   | K50   | 537 | G    |
| 1   | K50   | 540 | G    |
| 1   | K50   | 547 | U    |
| 1   | K50   | 549 | C    |
| 1   | K50   | 556 | A    |
| 1   | K50   | 557 | U    |
| 1   | K50   | 558 | A    |
| 1   | K50   | 563 | U    |
| 1   | K50   | 564 | G    |
| 1   | K50   | 568 | A    |
| 1   | K50   | 569 | C    |
| 1   | K50   | 570 | U    |
| 1   | K50   | 580 | U    |
| 1   | K50   | 581 | G    |
| 1   | K50   | 592 | U    |
| 1   | K50   | 603 | A    |
| 1   | K50   | 604 | G    |
| 1   | K50   | 608 | G    |
| 1   | K50   | 609 | A    |
| 1   | K50   | 612 | C    |
| 1   | K50   | 615 | C    |
| 1   | K50   | 625 | U    |
| 1   | K50   | 631 | G    |
| 1   | K50   | 645 | U    |
| 1   | K50   | 647 | A    |
| 1   | K50   | 648 | G    |
| 1   | K50   | 658 | G    |
| 1   | K50   | 659 | G    |
| 1   | K50   | 665 | A    |
| 1   | K50   | 666 | A    |
| 1   | K50   | 667 | G    |
| 1   | K50   | 668 | A    |
| 1   | K50   | 672 | A    |
| 1   | K50   | 675 | G    |
| 1   | K50   | 676 | A    |
| 1   | K50   | 685 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 688 | G    |
| 1   | K50   | 695 | C    |
| 1   | K50   | 704 | A    |
| 1   | K50   | 710 | A    |
| 1   | K50   | 711 | U    |
| 1   | K50   | 716 | A    |
| 1   | K50   | 720 | C    |
| 1   | K50   | 724 | C    |
| 1   | K50   | 726 | C    |
| 1   | K50   | 727 | G    |
| 1   | K50   | 729 | A    |
| 1   | K50   | 732 | G    |
| 1   | K50   | 735 | A    |
| 1   | K50   | 736 | A    |
| 1   | K50   | 737 | G    |
| 1   | K50   | 739 | A    |
| 1   | K50   | 742 | G    |
| 1   | K50   | 749 | A    |
| 1   | K50   | 763 | U    |
| 1   | K50   | 765 | A    |
| 1   | K50   | 766 | A    |
| 1   | K50   | 767 | G    |
| 1   | K50   | 772 | C    |
| 1   | K50   | 778 | A    |
| 1   | K50   | 782 | G    |
| 1   | K50   | 795 | U    |
| 1   | K50   | 797 | U    |
| 1   | K50   | 799 | C    |
| 1   | K50   | 801 | A    |
| 1   | K50   | 802 | U    |
| 1   | K50   | 803 | G    |
| 1   | K50   | 806 | A    |
| 1   | K50   | 816 | G    |
| 1   | K50   | 830 | G    |
| 1   | K50   | 834 | G    |
| 1   | K50   | 843 | A    |
| 1   | K50   | 848 | A    |
| 1   | K50   | 849 | A    |
| 1   | K50   | 852 | A    |
| 1   | K50   | 853 | A    |
| 1   | K50   | 854 | C    |
| 1   | K50   | 858 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 859 | C    |
| 1   | K50   | 860 | A    |
| 1   | K50   | 864 | U    |
| 1   | K50   | 865 | G    |
| 1   | K50   | 867 | U    |
| 1   | K50   | 872 | A    |
| 1   | K50   | 878 | A    |
| 1   | K50   | 879 | U    |
| 1   | K50   | 881 | U    |
| 1   | K50   | 885 | G    |
| 1   | K50   | 886 | A    |
| 1   | K50   | 889 | G    |
| 1   | K50   | 893 | C    |
| 1   | K50   | 899 | G    |
| 1   | K50   | 900 | A    |
| 1   | K50   | 905 | G    |
| 1   | K50   | 915 | G    |
| 1   | K50   | 916 | A    |
| 1   | K50   | 919 | G    |
| 1   | K50   | 921 | A    |
| 1   | K50   | 922 | G    |
| 1   | K50   | 925 | C    |
| 1   | K50   | 926 | G    |
| 1   | K50   | 927 | G    |
| 1   | K50   | 930 | G    |
| 1   | K50   | 931 | C    |
| 1   | K50   | 933 | A    |
| 1   | K50   | 934 | U    |
| 1   | K50   | 935 | G    |
| 1   | K50   | 936 | G    |
| 1   | K50   | 938 | A    |
| 1   | K50   | 939 | G    |
| 1   | K50   | 940 | U    |
| 1   | K50   | 941 | C    |
| 1   | K50   | 942 | G    |
| 1   | K50   | 945 | A    |
| 1   | K50   | 946 | U    |
| 1   | K50   | 947 | C    |
| 1   | K50   | 948 | C    |
| 1   | K50   | 949 | G    |
| 1   | K50   | 950 | G    |
| 1   | K50   | 951 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 953  | A    |
| 1   | K50   | 954  | G    |
| 1   | K50   | 955  | A    |
| 1   | K50   | 956  | A    |
| 1   | K50   | 957  | A    |
| 1   | K50   | 959  | G    |
| 1   | K50   | 961  | G    |
| 1   | K50   | 963  | U    |
| 1   | K50   | 964  | A    |
| 1   | K50   | 965  | C    |
| 1   | K50   | 966  | A    |
| 1   | K50   | 967  | A    |
| 1   | K50   | 968  | C    |
| 1   | K50   | 969  | G    |
| 1   | K50   | 970  | U    |
| 1   | K50   | 971  | A    |
| 1   | K50   | 972  | C    |
| 1   | K50   | 973  | C    |
| 1   | K50   | 975  | A    |
| 1   | K50   | 978  | G    |
| 1   | K50   | 980  | A    |
| 1   | K50   | 985  | U    |
| 1   | K50   | 988  | G    |
| 1   | K50   | 993  | G    |
| 1   | K50   | 998  | U    |
| 1   | K50   | 1000 | G    |
| 1   | K50   | 1001 | A    |
| 1   | K50   | 1002 | U    |
| 1   | K50   | 1006 | G    |
| 1   | K50   | 1010 | A    |
| 1   | K50   | 1012 | C    |
| 1   | K50   | 1015 | A    |
| 1   | K50   | 1018 | U    |
| 1   | K50   | 1019 | C    |
| 1   | K50   | 1021 | G    |
| 1   | K50   | 1022 | A    |
| 1   | K50   | 1024 | G    |
| 1   | K50   | 1032 | A    |
| 1   | K50   | 1034 | C    |
| 1   | K50   | 1036 | G    |
| 1   | K50   | 1047 | G    |
| 1   | K50   | 1050 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1053 | C    |
| 1   | K50   | 1059 | G    |
| 1   | K50   | 1061 | G    |
| 1   | K50   | 1067 | A    |
| 1   | K50   | 1068 | C    |
| 1   | K50   | 1075 | A    |
| 1   | K50   | 1076 | U    |
| 1   | K50   | 1084 | G    |
| 1   | K50   | 1085 | G    |
| 1   | K50   | 1087 | G    |
| 1   | K50   | 1092 | A    |
| 1   | K50   | 1096 | A    |
| 1   | K50   | 1097 | G    |
| 1   | K50   | 1099 | G    |
| 1   | K50   | 1101 | A    |
| 1   | K50   | 1102 | G    |
| 1   | K50   | 1104 | U    |
| 1   | K50   | 1105 | C    |
| 1   | K50   | 1111 | G    |
| 1   | K50   | 1116 | U    |
| 1   | K50   | 1117 | A    |
| 1   | K50   | 1120 | G    |
| 1   | K50   | 1121 | A    |
| 1   | K50   | 1123 | A    |
| 1   | K50   | 1124 | A    |
| 1   | K50   | 1130 | C    |
| 1   | K50   | 1131 | U    |
| 1   | K50   | 1133 | C    |
| 1   | K50   | 1135 | G    |
| 1   | K50   | 1136 | C    |
| 1   | K50   | 1140 | A    |
| 1   | K50   | 1141 | A    |
| 1   | K50   | 1142 | A    |
| 1   | K50   | 1144 | A    |
| 1   | K50   | 1148 | A    |
| 1   | K50   | 1149 | G    |
| 1   | K50   | 1150 | G    |
| 1   | K50   | 1155 | G    |
| 1   | K50   | 1163 | U    |
| 1   | K50   | 1169 | C    |
| 1   | K50   | 1170 | A    |
| 1   | K50   | 1171 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1172 | A    |
| 1   | K50   | 1173 | A    |
| 1   | K50   | 1176 | A    |
| 1   | K50   | 1177 | G    |
| 1   | K50   | 1181 | G    |
| 1   | K50   | 1182 | A    |
| 1   | K50   | 1183 | G    |
| 1   | K50   | 1185 | C    |
| 1   | K50   | 1189 | U    |
| 1   | K50   | 1192 | A    |
| 1   | K50   | 1198 | G    |
| 1   | K50   | 1204 | A    |
| 1   | K50   | 1206 | A    |
| 1   | K50   | 1217 | A    |
| 1   | K50   | 1218 | A    |
| 1   | K50   | 1223 | A    |
| 1   | K50   | 1226 | C    |
| 1   | K50   | 1227 | A    |
| 1   | K50   | 1229 | G    |
| 1   | K50   | 1231 | U    |
| 1   | K50   | 1232 | G    |
| 1   | K50   | 1233 | A    |
| 1   | K50   | 1235 | A    |
| 1   | K50   | 1236 | U    |
| 1   | K50   | 1237 | U    |
| 1   | K50   | 1247 | G    |
| 1   | K50   | 1250 | C    |
| 1   | K50   | 1254 | C    |
| 1   | K50   | 1257 | A    |
| 1   | K50   | 1264 | C    |
| 1   | K50   | 1268 | U    |
| 1   | K50   | 1270 | U    |
| 1   | K50   | 1271 | U    |
| 1   | K50   | 1273 | G    |
| 1   | K50   | 1274 | C    |
| 1   | K50   | 1278 | U    |
| 1   | K50   | 1281 | A    |
| 1   | K50   | 1283 | A    |
| 1   | K50   | 1308 | A    |
| 1   | K50   | 1309 | C    |
| 1   | K50   | 1318 | U    |
| 1   | K50   | 1327 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1332 | G    |
| 1   | K50   | 1339 | G    |
| 1   | K50   | 1340 | A    |
| 1   | K50   | 1341 | G    |
| 1   | K50   | 1342 | A    |
| 1   | K50   | 1346 | A    |
| 1   | K50   | 1351 | C    |
| 1   | K50   | 1360 | U    |
| 1   | K50   | 1374 | U    |
| 1   | K50   | 1375 | G    |
| 1   | K50   | 1383 | C    |
| 1   | K50   | 1385 | G    |
| 1   | K50   | 1387 | G    |
| 1   | K50   | 1388 | C    |
| 1   | K50   | 1391 | G    |
| 1   | K50   | 1393 | U    |
| 1   | K50   | 1395 | U    |
| 1   | K50   | 1396 | G    |
| 1   | K50   | 1400 | A    |
| 1   | K50   | 1411 | C    |
| 1   | K50   | 1412 | C    |
| 1   | K50   | 1414 | U    |
| 1   | K50   | 1415 | G    |
| 1   | K50   | 1416 | A    |
| 1   | K50   | 1417 | A    |
| 1   | K50   | 1421 | A    |
| 1   | K50   | 1427 | A    |
| 1   | K50   | 1429 | A    |
| 1   | K50   | 1430 | U    |
| 1   | K50   | 1431 | G    |
| 1   | K50   | 1437 | A    |
| 1   | K50   | 1441 | U    |
| 1   | K50   | 1449 | A    |
| 1   | K50   | 1450 | A    |
| 1   | K50   | 1454 | U    |
| 1   | K50   | 1457 | C    |
| 1   | K50   | 1458 | A    |
| 1   | K50   | 1463 | U    |
| 1   | K50   | 1465 | C    |
| 1   | K50   | 1466 | A    |
| 1   | K50   | 1468 | G    |
| 1   | K50   | 1474 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1485 | G    |
| 1   | K50   | 1486 | G    |
| 1   | K50   | 1488 | U    |
| 1   | K50   | 1489 | G    |
| 1   | K50   | 1490 | U    |
| 1   | K50   | 1491 | U    |
| 1   | K50   | 1492 | U    |
| 1   | K50   | 1499 | U    |
| 1   | K50   | 1500 | G    |
| 1   | K50   | 1503 | A    |
| 1   | K50   | 1504 | G    |
| 1   | K50   | 1506 | G    |
| 1   | K50   | 1513 | G    |
| 1   | K50   | 1527 | U    |
| 1   | K50   | 1535 | G    |
| 1   | K50   | 1536 | G    |
| 1   | K50   | 1539 | A    |
| 1   | K50   | 1547 | G    |
| 1   | K50   | 1554 | U    |
| 1   | K50   | 1555 | G    |
| 1   | K50   | 1556 | U    |
| 1   | K50   | 1557 | G    |
| 1   | K50   | 1563 | A    |
| 1   | K50   | 1564 | U    |
| 1   | K50   | 1565 | U    |
| 1   | K50   | 1571 | A    |
| 1   | K50   | 1573 | G    |
| 1   | K50   | 1574 | G    |
| 1   | K50   | 1583 | A    |
| 1   | K50   | 1592 | U    |
| 1   | K50   | 1603 | C    |
| 1   | K50   | 1609 | G    |
| 1   | K50   | 1610 | A    |
| 1   | K50   | 1611 | A    |
| 1   | K50   | 1612 | G    |
| 1   | K50   | 1613 | A    |
| 1   | K50   | 1614 | G    |
| 1   | K50   | 1619 | G    |
| 1   | K50   | 1625 | A    |
| 1   | K50   | 1626 | G    |
| 1   | K50   | 1628 | U    |
| 1   | K50   | 1629 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1643 | G    |
| 1   | K50   | 1645 | C    |
| 1   | K50   | 1649 | A    |
| 1   | K50   | 1651 | A    |
| 1   | K50   | 1653 | G    |
| 1   | K50   | 1668 | A    |
| 1   | K50   | 1675 | G    |
| 1   | K50   | 1679 | A    |
| 1   | K50   | 1680 | A    |
| 1   | K50   | 1685 | G    |
| 1   | K50   | 1687 | G    |
| 1   | K50   | 1688 | A    |
| 1   | K50   | 1692 | A    |
| 1   | K50   | 1693 | C    |
| 1   | K50   | 1700 | U    |
| 1   | K50   | 1705 | U    |
| 1   | K50   | 1706 | A    |
| 1   | K50   | 1708 | G    |
| 1   | K50   | 1709 | G    |
| 1   | K50   | 1715 | A    |
| 1   | K50   | 1717 | A    |
| 1   | K50   | 1718 | C    |
| 1   | K50   | 1720 | C    |
| 1   | K50   | 1723 | C    |
| 1   | K50   | 1724 | G    |
| 1   | K50   | 1731 | A    |
| 1   | K50   | 1733 | A    |
| 1   | K50   | 1734 | U    |
| 1   | K50   | 1739 | A    |
| 1   | K50   | 1740 | C    |
| 1   | K50   | 1742 | C    |
| 1   | K50   | 1743 | G    |
| 1   | K50   | 1744 | C    |
| 1   | K50   | 1746 | U    |
| 1   | K50   | 1749 | A    |
| 1   | K50   | 1751 | G    |
| 1   | K50   | 1753 | A    |
| 1   | K50   | 1754 | A    |
| 1   | K50   | 1755 | U    |
| 1   | K50   | 1756 | G    |
| 1   | K50   | 1760 | A    |
| 1   | K50   | 1771 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1772 | U    |
| 1   | K50   | 1797 | A    |
| 1   | K50   | 1801 | C    |
| 1   | K50   | 1803 | A    |
| 1   | K50   | 1808 | A    |
| 1   | K50   | 1809 | A    |
| 1   | K50   | 1810 | C    |
| 1   | K50   | 1811 | G    |
| 1   | K50   | 1828 | G    |
| 1   | K50   | 1832 | A    |
| 1   | K50   | 1836 | A    |
| 1   | K50   | 1837 | A    |
| 1   | K50   | 1838 | G    |
| 1   | K50   | 1839 | A    |
| 1   | K50   | 1846 | U    |
| 1   | K50   | 1854 | A    |
| 1   | K50   | 1862 | G    |
| 1   | K50   | 1869 | A    |
| 1   | K50   | 1876 | A    |
| 1   | K50   | 1880 | U    |
| 1   | K50   | 1882 | G    |
| 1   | K50   | 1883 | A    |
| 1   | K50   | 1884 | G    |
| 1   | K50   | 1885 | G    |
| 1   | K50   | 1886 | C    |
| 1   | K50   | 1887 | G    |
| 1   | K50   | 1889 | U    |
| 1   | K50   | 1890 | G    |
| 1   | K50   | 1893 | G    |
| 1   | K50   | 1895 | A    |
| 1   | K50   | 1896 | A    |
| 1   | K50   | 1897 | G    |
| 1   | K50   | 1898 | G    |
| 1   | K50   | 1899 | U    |
| 1   | K50   | 1902 | A    |
| 1   | K50   | 1903 | G    |
| 1   | K50   | 1905 | G    |
| 1   | K50   | 1912 | C    |
| 1   | K50   | 1915 | A    |
| 1   | K50   | 1916 | A    |
| 1   | K50   | 1917 | G    |
| 1   | K50   | 1919 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1920 | A    |
| 1   | K50   | 1921 | A    |
| 1   | K50   | 1923 | G    |
| 1   | K50   | 1927 | A    |
| 1   | K50   | 1928 | C    |
| 1   | K50   | 1929 | U    |
| 1   | K50   | 1930 | G    |
| 1   | K50   | 1931 | C    |
| 1   | K50   | 1933 | C    |
| 1   | K50   | 1934 | C    |
| 1   | K50   | 1937 | G    |
| 1   | K50   | 1939 | U    |
| 1   | K50   | 1940 | C    |
| 1   | K50   | 1947 | A    |
| 1   | K50   | 1950 | C    |
| 1   | K50   | 1951 | A    |
| 1   | K50   | 1953 | U    |
| 1   | K50   | 1956 | U    |
| 1   | K50   | 1957 | U    |
| 1   | K50   | 1958 | U    |
| 1   | K50   | 1959 | A    |
| 1   | K50   | 1961 | G    |
| 1   | K50   | 1962 | G    |
| 1   | K50   | 1963 | A    |
| 1   | K50   | 1964 | C    |
| 1   | K50   | 1967 | A    |
| 1   | K50   | 1977 | G    |
| 1   | K50   | 1978 | G    |
| 1   | K50   | 1983 | U    |
| 1   | K50   | 1985 | G    |
| 1   | K50   | 1990 | G    |
| 1   | K50   | 1991 | G    |
| 1   | K50   | 1995 | G    |
| 1   | K50   | 1997 | A    |
| 1   | K50   | 1999 | G    |
| 1   | K50   | 2008 | A    |
| 1   | K50   | 2011 | A    |
| 1   | K50   | 2013 | A    |
| 1   | K50   | 2019 | G    |
| 1   | K50   | 2023 | A    |
| 1   | K50   | 2027 | A    |
| 1   | K50   | 2028 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2036 | A    |
| 1   | K50   | 2037 | C    |
| 1   | K50   | 2039 | G    |
| 1   | K50   | 2042 | A    |
| 1   | K50   | 2043 | G    |
| 1   | K50   | 2044 | A    |
| 1   | K50   | 2045 | C    |
| 1   | K50   | 2046 | G    |
| 1   | K50   | 2047 | A    |
| 1   | K50   | 2048 | G    |
| 1   | K50   | 2053 | C    |
| 1   | K50   | 2054 | U    |
| 1   | K50   | 2055 | C    |
| 1   | K50   | 2057 | U    |
| 1   | K50   | 2059 | U    |
| 1   | K50   | 2060 | A    |
| 1   | K50   | 2061 | G    |
| 1   | K50   | 2062 | A    |
| 1   | K50   | 2067 | A    |
| 1   | K50   | 2073 | U    |
| 1   | K50   | 2075 | A    |
| 1   | K50   | 2076 | A    |
| 1   | K50   | 2077 | G    |
| 1   | K50   | 2078 | A    |
| 1   | K50   | 2079 | G    |
| 1   | K50   | 2085 | G    |
| 1   | K50   | 2087 | G    |
| 1   | K50   | 2093 | G    |
| 1   | K50   | 2098 | A    |
| 1   | K50   | 2109 | G    |
| 1   | K50   | 2110 | A    |
| 1   | K50   | 2111 | G    |
| 1   | K50   | 2122 | G    |
| 1   | K50   | 2124 | C    |
| 1   | K50   | 2130 | G    |
| 1   | K50   | 2131 | A    |
| 1   | K50   | 2136 | A    |
| 1   | K50   | 2140 | A    |
| 1   | K50   | 2141 | U    |
| 1   | K50   | 2142 | A    |
| 1   | K50   | 2145 | A    |
| 1   | K50   | 2152 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2159 | U    |
| 1   | K50   | 2164 | G    |
| 1   | K50   | 2168 | G    |
| 1   | K50   | 2169 | A    |
| 1   | K50   | 2170 | A    |
| 1   | K50   | 2178 | C    |
| 1   | K50   | 2184 | G    |
| 1   | K50   | 2185 | A    |
| 1   | K50   | 2206 | A    |
| 1   | K50   | 2210 | U    |
| 1   | K50   | 2211 | A    |
| 1   | K50   | 2213 | A    |
| 1   | K50   | 2218 | G    |
| 1   | K50   | 2221 | G    |
| 1   | K50   | 2227 | U    |
| 1   | K50   | 2228 | U    |
| 1   | K50   | 2229 | U    |
| 1   | K50   | 2235 | C    |
| 1   | K50   | 2239 | G    |
| 1   | K50   | 2243 | U    |
| 1   | K50   | 2253 | C    |
| 1   | K50   | 2255 | A    |
| 1   | K50   | 2260 | G    |
| 1   | K50   | 2262 | C    |
| 1   | K50   | 2266 | G    |
| 1   | K50   | 2267 | C    |
| 1   | K50   | 2268 | A    |
| 1   | K50   | 2269 | G    |
| 1   | K50   | 2270 | C    |
| 1   | K50   | 2272 | G    |
| 1   | K50   | 2279 | A    |
| 1   | K50   | 2282 | G    |
| 1   | K50   | 2291 | U    |
| 1   | K50   | 2296 | C    |
| 1   | K50   | 2303 | C    |
| 1   | K50   | 2304 | A    |
| 1   | K50   | 2309 | A    |
| 1   | K50   | 2310 | C    |
| 1   | K50   | 2313 | G    |
| 1   | K50   | 2319 | G    |
| 1   | K50   | 2322 | U    |
| 1   | K50   | 2323 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2325 | G    |
| 1   | K50   | 2335 | A    |
| 1   | K50   | 2339 | A    |
| 1   | K50   | 2340 | G    |
| 1   | K50   | 2345 | G    |
| 1   | K50   | 2351 | U    |
| 1   | K50   | 2355 | A    |
| 1   | K50   | 2360 | C    |
| 1   | K50   | 2366 | A    |
| 1   | K50   | 2368 | U    |
| 1   | K50   | 2376 | A    |
| 1   | K50   | 2377 | G    |
| 1   | K50   | 2379 | G    |
| 1   | K50   | 2388 | U    |
| 1   | K50   | 2391 | G    |
| 1   | K50   | 2401 | C    |
| 1   | K50   | 2420 | C    |
| 1   | K50   | 2423 | C    |
| 1   | K50   | 2428 | G    |
| 1   | K50   | 2435 | A    |
| 1   | K50   | 2436 | G    |
| 1   | K50   | 2441 | A    |
| 1   | K50   | 2447 | A    |
| 1   | K50   | 2453 | C    |
| 1   | K50   | 2454 | G    |
| 1   | K50   | 2458 | C    |
| 1   | K50   | 2459 | C    |
| 1   | K50   | 2460 | U    |
| 1   | K50   | 2467 | U    |
| 1   | K50   | 2469 | G    |
| 1   | K50   | 2470 | C    |
| 1   | K50   | 2471 | U    |
| 1   | K50   | 2473 | G    |
| 1   | K50   | 2474 | A    |
| 1   | K50   | 2477 | C    |
| 1   | K50   | 2478 | C    |
| 1   | K50   | 2480 | C    |
| 1   | K50   | 2481 | U    |
| 1   | K50   | 2482 | A    |
| 1   | K50   | 2483 | A    |
| 1   | K50   | 2487 | A    |
| 1   | K50   | 2488 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2490 | A    |
| 1   | K50   | 2491 | A    |
| 1   | K50   | 2501 | A    |
| 1   | K50   | 2519 | G    |
| 1   | K50   | 2520 | A    |
| 1   | K50   | 2534 | U    |
| 1   | K50   | 2535 | U    |
| 1   | K50   | 2539 | A    |
| 1   | K50   | 2540 | G    |
| 1   | K50   | 2542 | G    |
| 1   | K50   | 2543 | G    |
| 1   | K50   | 2549 | U    |
| 1   | K50   | 2553 | A    |
| 1   | K50   | 2561 | U    |
| 1   | K50   | 2562 | U    |
| 1   | K50   | 2563 | U    |
| 1   | K50   | 2568 | U    |
| 1   | K50   | 2582 | G    |
| 1   | K50   | 2588 | G    |
| 1   | K50   | 2595 | U    |
| 1   | K50   | 2596 | G    |
| 1   | K50   | 2598 | U    |
| 1   | K50   | 2599 | U    |
| 1   | K50   | 2606 | A    |
| 2   | R60   | 2    | C    |
| 2   | R60   | 3    | C    |
| 2   | R60   | 7    | U    |
| 2   | R60   | 8    | U    |
| 2   | R60   | 18   | U    |
| 2   | R60   | 32   | G    |
| 2   | R60   | 33   | U    |
| 2   | R60   | 35   | U    |
| 2   | R60   | 39   | A    |
| 2   | R60   | 40   | G    |
| 2   | R60   | 41   | A    |
| 2   | R60   | 43   | U    |
| 2   | R60   | 45   | A    |
| 2   | R60   | 48   | C    |
| 2   | R60   | 54   | U    |
| 2   | R60   | 55   | G    |
| 2   | R60   | 56   | U    |
| 2   | R60   | 57   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R60   | 58  | U    |
| 2   | R60   | 59  | A    |
| 2   | R60   | 61  | G    |
| 2   | R60   | 62  | C    |
| 2   | R60   | 63  | G    |
| 2   | R60   | 64  | A    |
| 2   | R60   | 65  | A    |
| 2   | R60   | 66  | G    |
| 2   | R60   | 68  | G    |
| 2   | R60   | 69  | A    |
| 2   | R60   | 71  | U    |
| 2   | R60   | 72  | A    |
| 2   | R60   | 74  | U    |
| 2   | R60   | 75  | G    |
| 2   | R60   | 76  | A    |
| 2   | R60   | 77  | A    |
| 2   | R60   | 78  | G    |
| 2   | R60   | 79  | C    |
| 2   | R60   | 80  | G    |
| 2   | R60   | 84  | G    |
| 2   | R60   | 85  | A    |
| 2   | R60   | 86  | A    |
| 2   | R60   | 92  | A    |
| 2   | R60   | 94  | U    |
| 2   | R60   | 96  | A    |
| 2   | R60   | 97  | C    |
| 2   | R60   | 106 | A    |
| 2   | R60   | 107 | U    |
| 2   | R60   | 116 | U    |
| 2   | R60   | 118 | G    |
| 2   | R60   | 119 | A    |
| 2   | R60   | 121 | C    |
| 2   | R60   | 127 | A    |
| 2   | R60   | 128 | A    |
| 2   | R60   | 130 | C    |
| 2   | R60   | 133 | A    |
| 2   | R60   | 134 | G    |
| 2   | R60   | 135 | G    |
| 2   | R60   | 136 | A    |
| 2   | R60   | 137 | A    |
| 2   | R60   | 138 | A    |
| 2   | R60   | 140 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R60   | 141 | G    |
| 2   | R60   | 142 | A    |
| 2   | R60   | 143 | G    |
| 2   | R60   | 144 | G    |
| 2   | R60   | 149 | A    |
| 2   | R60   | 150 | A    |
| 2   | R60   | 181 | A    |
| 2   | R60   | 183 | G    |
| 2   | R60   | 184 | A    |
| 2   | R60   | 186 | A    |
| 2   | R60   | 187 | A    |
| 2   | R60   | 188 | C    |
| 2   | R60   | 190 | A    |
| 2   | R60   | 191 | C    |
| 2   | R60   | 193 | G    |
| 2   | R60   | 194 | U    |
| 2   | R60   | 195 | G    |
| 2   | R60   | 197 | A    |
| 2   | R60   | 204 | U    |
| 2   | R60   | 205 | A    |
| 2   | R60   | 214 | U    |
| 2   | R60   | 215 | C    |
| 2   | R60   | 220 | C    |
| 2   | R60   | 221 | A    |
| 2   | R60   | 222 | G    |
| 2   | R60   | 226 | G    |
| 2   | R60   | 241 | G    |
| 2   | R60   | 242 | C    |
| 2   | R60   | 247 | U    |
| 2   | R60   | 255 | A    |
| 2   | R60   | 256 | G    |
| 2   | R60   | 263 | A    |
| 2   | R60   | 264 | C    |
| 2   | R60   | 266 | G    |
| 2   | R60   | 268 | G    |
| 2   | R60   | 280 | G    |
| 2   | R60   | 281 | A    |
| 2   | R60   | 283 | U    |
| 2   | R60   | 284 | C    |
| 2   | R60   | 287 | G    |
| 2   | R60   | 288 | A    |
| 2   | R60   | 289 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R60   | 302 | A    |
| 2   | R60   | 303 | G    |
| 2   | R60   | 304 | A    |
| 2   | R60   | 305 | C    |
| 2   | R60   | 306 | G    |
| 2   | R60   | 307 | G    |
| 2   | R60   | 309 | U    |
| 2   | R60   | 310 | A    |
| 2   | R60   | 311 | C    |
| 2   | R60   | 315 | G    |
| 2   | R60   | 317 | C    |
| 2   | R60   | 318 | C    |
| 2   | R60   | 319 | A    |
| 2   | R60   | 320 | A    |
| 2   | R60   | 321 | G    |
| 2   | R60   | 327 | C    |
| 2   | R60   | 328 | A    |
| 2   | R60   | 329 | G    |
| 2   | R60   | 331 | A    |
| 2   | R60   | 337 | G    |
| 2   | R60   | 339 | A    |
| 2   | R60   | 340 | A    |
| 2   | R60   | 341 | A    |
| 2   | R60   | 342 | U    |
| 2   | R60   | 343 | U    |
| 2   | R60   | 347 | G    |
| 2   | R60   | 355 | C    |
| 2   | R60   | 356 | A    |
| 2   | R60   | 357 | A    |
| 2   | R60   | 358 | G    |
| 2   | R60   | 362 | G    |
| 2   | R60   | 363 | C    |
| 2   | R60   | 364 | G    |
| 2   | R60   | 371 | A    |
| 2   | R60   | 372 | A    |
| 2   | R60   | 378 | G    |
| 2   | R60   | 380 | G    |
| 2   | R60   | 383 | A    |
| 2   | R60   | 384 | A    |
| 2   | R60   | 385 | C    |
| 2   | R60   | 387 | A    |
| 2   | R60   | 388 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R60   | 389 | U    |
| 2   | R60   | 390 | G    |
| 2   | R60   | 391 | U    |
| 2   | R60   | 392 | G    |
| 2   | R60   | 393 | U    |
| 2   | R60   | 394 | G    |
| 2   | R60   | 398 | A    |
| 2   | R60   | 400 | A    |
| 2   | R60   | 401 | C    |
| 2   | R60   | 403 | A    |
| 2   | R60   | 404 | C    |
| 2   | R60   | 406 | U    |
| 2   | R60   | 407 | G    |
| 2   | R60   | 408 | A    |
| 2   | R60   | 409 | G    |
| 2   | R60   | 414 | U    |
| 2   | R60   | 416 | G    |
| 2   | R60   | 418 | G    |
| 2   | R60   | 420 | U    |
| 2   | R60   | 421 | C    |
| 2   | R60   | 422 | A    |
| 2   | R60   | 424 | G    |
| 2   | R60   | 425 | G    |
| 2   | R60   | 426 | C    |
| 2   | R60   | 429 | G    |
| 2   | R60   | 430 | U    |
| 2   | R60   | 431 | G    |
| 2   | R60   | 432 | C    |
| 2   | R60   | 434 | A    |
| 2   | R60   | 435 | G    |
| 2   | R60   | 437 | A    |
| 2   | R60   | 438 | U    |
| 2   | R60   | 439 | C    |
| 2   | R60   | 440 | C    |
| 2   | R60   | 441 | G    |
| 2   | R60   | 443 | G    |
| 2   | R60   | 444 | G    |
| 2   | R60   | 445 | U    |
| 2   | R60   | 446 | A    |
| 2   | R60   | 447 | A    |
| 2   | R60   | 448 | U    |
| 2   | R60   | 449 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R60   | 450 | C    |
| 2   | R60   | 451 | C    |
| 2   | R60   | 452 | A    |
| 2   | R60   | 453 | G    |
| 2   | R60   | 461 | A    |
| 2   | R60   | 462 | G    |
| 2   | R60   | 463 | U    |
| 2   | R60   | 465 | U    |
| 2   | R60   | 468 | A    |
| 2   | R60   | 474 | A    |
| 2   | R60   | 477 | G    |
| 2   | R60   | 478 | C    |
| 2   | R60   | 484 | U    |
| 2   | R60   | 486 | A    |
| 2   | R60   | 487 | A    |
| 2   | R60   | 490 | G    |
| 2   | R60   | 499 | U    |
| 2   | R60   | 501 | G    |
| 2   | R60   | 502 | A    |
| 2   | R60   | 505 | A    |
| 2   | R60   | 506 | A    |
| 2   | R60   | 507 | C    |
| 2   | R60   | 510 | U    |
| 2   | R60   | 512 | C    |
| 2   | R60   | 520 | U    |
| 2   | R60   | 521 | A    |
| 2   | R60   | 523 | U    |
| 2   | R60   | 524 | G    |
| 2   | R60   | 527 | G    |
| 2   | R60   | 535 | A    |
| 2   | R60   | 540 | C    |
| 2   | R60   | 554 | A    |
| 2   | R60   | 562 | G    |
| 2   | R60   | 565 | U    |
| 2   | R60   | 566 | A    |
| 2   | R60   | 567 | A    |
| 2   | R60   | 568 | G    |
| 2   | R60   | 570 | A    |
| 2   | R60   | 578 | A    |
| 2   | R60   | 581 | G    |
| 2   | R60   | 582 | C    |
| 2   | R60   | 587 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R60   | 590 | U    |
| 2   | R60   | 593 | A    |
| 2   | R60   | 599 | G    |
| 2   | R60   | 600 | A    |
| 2   | R60   | 601 | G    |
| 2   | R60   | 608 | A    |
| 2   | R60   | 609 | A    |
| 2   | R60   | 610 | U    |
| 2   | R60   | 621 | G    |
| 2   | R60   | 622 | C    |
| 2   | R60   | 623 | U    |
| 2   | R60   | 624 | U    |
| 2   | R60   | 627 | G    |
| 2   | R60   | 635 | G    |
| 2   | R60   | 646 | G    |
| 2   | R60   | 647 | C    |
| 2   | R60   | 653 | A    |
| 2   | R60   | 662 | U    |
| 2   | R60   | 668 | G    |
| 2   | R60   | 676 | A    |
| 2   | R60   | 680 | A    |
| 2   | R60   | 685 | G    |
| 2   | R60   | 686 | G    |
| 2   | R60   | 687 | A    |
| 2   | R60   | 690 | A    |
| 2   | R60   | 694 | A    |
| 2   | R60   | 700 | A    |
| 2   | R60   | 702 | U    |
| 2   | R60   | 703 | A    |
| 2   | R60   | 705 | A    |
| 2   | R60   | 707 | A    |
| 2   | R60   | 712 | A    |
| 2   | R60   | 714 | U    |
| 2   | R60   | 716 | G    |
| 2   | R60   | 722 | G    |
| 2   | R60   | 728 | A    |
| 2   | R60   | 730 | C    |
| 2   | R60   | 731 | G    |
| 2   | R60   | 732 | A    |
| 2   | R60   | 733 | U    |
| 2   | R60   | 734 | G    |
| 2   | R60   | 736 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R60   | 738 | A    |
| 2   | R60   | 739 | C    |
| 2   | R60   | 740 | G    |
| 2   | R60   | 749 | G    |
| 2   | R60   | 752 | A    |
| 2   | R60   | 754 | G    |
| 2   | R60   | 755 | A    |
| 2   | R60   | 756 | G    |
| 2   | R60   | 760 | G    |
| 2   | R60   | 768 | A    |
| 2   | R60   | 775 | U    |
| 2   | R60   | 776 | A    |
| 2   | R60   | 777 | G    |
| 2   | R60   | 778 | U    |
| 2   | R60   | 780 | G    |
| 2   | R60   | 781 | G    |
| 2   | R60   | 788 | G    |
| 2   | R60   | 806 | G    |
| 2   | R60   | 808 | G    |
| 2   | R60   | 812 | A    |
| 2   | R60   | 817 | A    |
| 2   | R60   | 818 | A    |
| 2   | R60   | 820 | G    |
| 2   | R60   | 824 | A    |
| 2   | R60   | 826 | U    |
| 2   | R60   | 828 | A    |
| 2   | R60   | 830 | G    |
| 2   | R60   | 831 | G    |
| 2   | R60   | 832 | A    |
| 2   | R60   | 833 | A    |
| 2   | R60   | 835 | A    |
| 2   | R60   | 836 | A    |
| 2   | R60   | 839 | C    |
| 2   | R60   | 840 | C    |
| 2   | R60   | 841 | A    |
| 2   | R60   | 849 | U    |
| 2   | R60   | 852 | A    |
| 2   | R60   | 854 | U    |
| 2   | R60   | 866 | U    |
| 2   | R60   | 868 | U    |
| 2   | R60   | 872 | U    |
| 2   | R60   | 873 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R60   | 874 | A    |
| 2   | R60   | 875 | A    |
| 2   | R60   | 877 | G    |
| 2   | R60   | 878 | C    |
| 2   | R60   | 879 | G    |
| 2   | R60   | 880 | G    |
| 2   | R60   | 883 | C    |
| 2   | R60   | 884 | A    |
| 2   | R60   | 887 | U    |
| 2   | R60   | 890 | C    |
| 2   | R60   | 898 | G    |
| 2   | R60   | 899 | A    |
| 2   | R60   | 906 | U    |
| 2   | R60   | 908 | U    |
| 2   | R60   | 909 | G    |
| 2   | R60   | 911 | G    |
| 2   | R60   | 912 | C    |
| 2   | R60   | 913 | G    |
| 2   | R60   | 914 | U    |
| 2   | R60   | 915 | A    |
| 2   | R60   | 916 | G    |
| 2   | R60   | 917 | U    |
| 2   | R60   | 918 | A    |
| 2   | R60   | 919 | C    |
| 2   | R60   | 921 | C    |
| 2   | R60   | 922 | G    |
| 2   | R60   | 924 | U    |
| 2   | R60   | 925 | A    |
| 2   | R60   | 926 | G    |
| 2   | R60   | 927 | G    |
| 2   | R60   | 929 | C    |
| 2   | R60   | 937 | G    |
| 2   | R60   | 941 | C    |
| 2   | R60   | 947 | C    |
| 2   | R60   | 948 | G    |
| 2   | R60   | 950 | U    |
| 2   | R60   | 952 | A    |
| 2   | R60   | 953 | C    |
| 2   | R60   | 955 | A    |
| 2   | R60   | 957 | G    |
| 2   | R60   | 959 | G    |
| 2   | R60   | 960 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | R60   | 968  | C    |
| 2   | R60   | 969  | C    |
| 2   | R60   | 970  | U    |
| 2   | R60   | 971  | U    |
| 2   | R60   | 972  | U    |
| 2   | R60   | 974  | G    |
| 2   | R60   | 980  | G    |
| 2   | R60   | 981  | U    |
| 2   | R60   | 985  | C    |
| 2   | R60   | 986  | G    |
| 2   | R60   | 987  | A    |
| 2   | R60   | 988  | A    |
| 2   | R60   | 989  | G    |
| 2   | R60   | 990  | U    |
| 2   | R60   | 992  | G    |
| 2   | R60   | 995  | A    |
| 2   | R60   | 996  | G    |
| 2   | R60   | 998  | U    |
| 2   | R60   | 1000 | C    |
| 2   | R60   | 1001 | C    |
| 2   | R60   | 1003 | A    |
| 2   | R60   | 1004 | G    |
| 2   | R60   | 1005 | G    |
| 2   | R60   | 1006 | A    |
| 2   | R60   | 1011 | A    |
| 2   | R60   | 1012 | A    |
| 2   | R60   | 1013 | A    |
| 2   | R60   | 1014 | G    |
| 2   | R60   | 1017 | A    |
| 2   | R60   | 1018 | U    |
| 2   | R60   | 1019 | C    |
| 2   | R60   | 1021 | A    |
| 2   | R60   | 1022 | C    |
| 2   | R60   | 1023 | A    |
| 2   | R60   | 1024 | G    |
| 2   | R60   | 1028 | U    |
| 2   | R60   | 1029 | U    |
| 2   | R60   | 1030 | A    |
| 2   | R60   | 1031 | A    |
| 2   | R60   | 1033 | A    |
| 2   | R60   | 1034 | A    |
| 2   | R60   | 1037 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | R60   | 1039 | G    |
| 2   | R60   | 1040 | G    |
| 2   | R60   | 1041 | A    |
| 2   | R60   | 1042 | A    |
| 2   | R60   | 1043 | G    |
| 2   | R60   | 1044 | G    |
| 2   | R60   | 1045 | A    |
| 2   | R60   | 1046 | A    |
| 2   | R60   | 1047 | G    |
| 2   | R60   | 1048 | G    |
| 2   | R60   | 1049 | G    |
| 2   | R60   | 1050 | G    |
| 2   | R60   | 1051 | C    |
| 2   | R60   | 1052 | A    |
| 2   | R60   | 1053 | A    |
| 2   | R60   | 1055 | A    |
| 2   | R60   | 1056 | A    |
| 2   | R60   | 1057 | C    |
| 2   | R60   | 1058 | A    |
| 2   | R60   | 1059 | G    |
| 2   | R60   | 1060 | G    |
| 2   | R60   | 1061 | U    |
| 2   | R60   | 1062 | C    |
| 2   | R60   | 1063 | A    |
| 2   | R60   | 1064 | G    |
| 2   | R60   | 1065 | U    |
| 2   | R60   | 1066 | G    |
| 2   | R60   | 1067 | A    |
| 2   | R60   | 1071 | C    |
| 2   | R60   | 1073 | U    |
| 2   | R60   | 1075 | A    |
| 2   | R60   | 1076 | G    |
| 2   | R60   | 1077 | A    |
| 2   | R60   | 1083 | U    |
| 2   | R60   | 1084 | G    |
| 2   | R60   | 1085 | G    |
| 2   | R60   | 1089 | G    |
| 2   | R60   | 1090 | C    |
| 2   | R60   | 1091 | A    |
| 2   | R60   | 1094 | C    |
| 2   | R60   | 1096 | C    |
| 2   | R60   | 1097 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | R60   | 1100 | A    |
| 2   | R60   | 1102 | A    |
| 2   | R60   | 1103 | G    |
| 2   | R60   | 1105 | G    |
| 2   | R60   | 1110 | C    |
| 2   | R60   | 1113 | C    |
| 2   | R60   | 1114 | A    |
| 2   | R60   | 1116 | A    |
| 2   | R60   | 1117 | A    |
| 2   | R60   | 1118 | A    |
| 2   | R60   | 1119 | C    |
| 2   | R60   | 1120 | A    |
| 2   | R60   | 1121 | A    |
| 2   | R60   | 1122 | A    |
| 2   | R60   | 1123 | U    |
| 2   | R60   | 1124 | A    |
| 2   | R60   | 1125 | G    |
| 2   | R60   | 1126 | A    |
| 2   | R60   | 1127 | A    |
| 2   | R60   | 1130 | A    |
| 2   | R60   | 1132 | A    |
| 2   | R60   | 1133 | U    |
| 2   | R60   | 1136 | G    |
| 2   | R60   | 1137 | A    |
| 2   | R60   | 1138 | U    |
| 2   | R60   | 1139 | C    |
| 2   | R60   | 1141 | A    |
| 2   | R60   | 1142 | G    |
| 2   | R60   | 1143 | A    |
| 2   | R60   | 1146 | G    |
| 2   | R60   | 1155 | C    |
| 2   | R60   | 1158 | U    |
| 2   | R60   | 1161 | U    |
| 2   | R60   | 1164 | G    |
| 2   | R60   | 1165 | C    |
| 2   | R60   | 1166 | A    |
| 2   | R60   | 1168 | A    |
| 2   | R60   | 1169 | G    |
| 2   | R60   | 1171 | A    |
| 2   | R60   | 1173 | C    |
| 2   | R60   | 1178 | A    |
| 2   | R60   | 1182 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | R60   | 1185 | A    |
| 2   | R60   | 1190 | U    |
| 2   | R60   | 1191 | C    |
| 2   | R60   | 1192 | G    |
| 2   | R60   | 1193 | U    |
| 2   | R60   | 1195 | A    |
| 2   | R60   | 1197 | C    |
| 2   | R60   | 1198 | U    |
| 2   | R60   | 1199 | C    |
| 2   | R60   | 1200 | A    |
| 2   | R60   | 1202 | U    |
| 2   | R60   | 1203 | A    |
| 2   | R60   | 1204 | A    |
| 2   | R60   | 1205 | G    |
| 2   | R60   | 1206 | A    |
| 2   | R60   | 1207 | A    |
| 2   | R60   | 1208 | G    |
| 2   | R60   | 1209 | C    |
| 2   | R60   | 1210 | G    |
| 2   | R60   | 1211 | A    |
| 2   | R60   | 1214 | A    |
| 2   | R60   | 1215 | A    |
| 2   | R60   | 1216 | U    |
| 2   | R60   | 1217 | G    |
| 2   | R60   | 1221 | C    |
| 2   | R60   | 1223 | C    |
| 2   | R60   | 1225 | G    |
| 2   | R60   | 1230 | U    |
| 2   | R60   | 1232 | G    |
| 2   | R60   | 1233 | U    |
| 2   | R60   | 1237 | C    |
| 2   | R60   | 1239 | C    |
| 2   | R60   | 1240 | C    |
| 2   | R60   | 1248 | G    |
| 2   | R60   | 1250 | U    |
| 2   | R60   | 1251 | A    |
| 2   | R60   | 1260 | G    |
| 2   | R60   | 1262 | A    |
| 2   | R60   | 1263 | A    |
| 2   | R60   | 1266 | A    |
| 2   | R60   | 1267 | G    |
| 2   | R60   | 1274 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | R60   | 1283 | A    |
| 2   | R60   | 1284 | G    |
| 2   | R60   | 1287 | A    |
| 2   | R60   | 1291 | A    |
| 2   | R60   | 1292 | G    |
| 2   | R60   | 1294 | G    |
| 2   | R60   | 1295 | C    |
| 2   | R60   | 1296 | A    |
| 2   | R60   | 1297 | G    |
| 2   | R60   | 1298 | G    |
| 2   | R60   | 1300 | U    |
| 2   | R60   | 1301 | U    |
| 2   | R60   | 1302 | C    |
| 2   | R60   | 1303 | U    |
| 2   | R60   | 1308 | C    |
| 2   | R60   | 1310 | G    |
| 2   | R60   | 1312 | U    |
| 2   | R60   | 1313 | A    |
| 2   | R60   | 1314 | C    |
| 2   | R60   | 1315 | A    |
| 2   | R60   | 1316 | A    |
| 2   | R60   | 1317 | G    |
| 2   | R60   | 1319 | C    |
| 2   | R60   | 1320 | G    |
| 2   | R60   | 1322 | A    |
| 2   | R60   | 1325 | A    |
| 2   | R60   | 1326 | A    |
| 2   | R60   | 1327 | G    |
| 2   | R60   | 1328 | G    |
| 2   | R60   | 1329 | C    |
| 2   | R60   | 1340 | G    |
| 2   | R60   | 1342 | A    |
| 2   | R60   | 1343 | C    |
| 2   | R60   | 1346 | G    |
| 2   | R60   | 1352 | G    |
| 2   | R60   | 1354 | A    |
| 2   | R60   | 1355 | U    |
| 2   | R60   | 1356 | C    |
| 2   | R60   | 1357 | A    |
| 7   | K70   | 2    | G    |
| 7   | K70   | 3    | U    |
| 7   | K70   | 4    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | K70   | 5   | A    |
| 7   | K70   | 7   | G    |
| 7   | K70   | 14  | U    |
| 7   | K70   | 17  | A    |
| 7   | K70   | 22  | A    |
| 7   | K70   | 26  | C    |
| 7   | K70   | 27  | A    |
| 7   | K70   | 28  | C    |
| 7   | K70   | 29  | C    |
| 7   | K70   | 33  | U    |
| 7   | K70   | 34  | C    |
| 7   | K70   | 41  | G    |
| 7   | K70   | 42  | A    |
| 7   | K70   | 45  | U    |
| 7   | K70   | 49  | A    |
| 7   | K70   | 50  | A    |
| 7   | K70   | 54  | A    |
| 7   | K70   | 55  | A    |
| 7   | K70   | 63  | A    |
| 7   | K70   | 64  | G    |
| 7   | K70   | 67  | C    |
| 7   | K70   | 76  | U    |
| 7   | K70   | 91  | C    |
| 7   | K70   | 100 | A    |
| 7   | K70   | 101 | A    |
| 7   | K70   | 110 | G    |
| 1   | L50   | 2   | U    |
| 1   | L50   | 3   | A    |
| 1   | L50   | 14  | G    |
| 1   | L50   | 15  | G    |
| 1   | L50   | 16  | G    |
| 1   | L50   | 17  | A    |
| 1   | L50   | 22  | U    |
| 1   | L50   | 23  | U    |
| 1   | L50   | 24  | G    |
| 1   | L50   | 43  | G    |
| 1   | L50   | 47  | C    |
| 1   | L50   | 48  | A    |
| 1   | L50   | 49  | G    |
| 1   | L50   | 50  | C    |
| 1   | L50   | 52  | G    |
| 1   | L50   | 59  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 61  | A    |
| 1   | L50   | 62  | U    |
| 1   | L50   | 68  | G    |
| 1   | L50   | 70  | A    |
| 1   | L50   | 71  | G    |
| 1   | L50   | 73  | A    |
| 1   | L50   | 75  | C    |
| 1   | L50   | 76  | A    |
| 1   | L50   | 87  | C    |
| 1   | L50   | 88  | A    |
| 1   | L50   | 97  | A    |
| 1   | L50   | 99  | U    |
| 1   | L50   | 100 | A    |
| 1   | L50   | 110 | G    |
| 1   | L50   | 111 | C    |
| 1   | L50   | 112 | U    |
| 1   | L50   | 114 | G    |
| 1   | L50   | 118 | A    |
| 1   | L50   | 123 | U    |
| 1   | L50   | 124 | U    |
| 1   | L50   | 132 | A    |
| 1   | L50   | 134 | C    |
| 1   | L50   | 135 | A    |
| 1   | L50   | 139 | G    |
| 1   | L50   | 149 | A    |
| 1   | L50   | 151 | G    |
| 1   | L50   | 152 | A    |
| 1   | L50   | 156 | G    |
| 1   | L50   | 157 | A    |
| 1   | L50   | 158 | A    |
| 1   | L50   | 159 | A    |
| 1   | L50   | 160 | C    |
| 1   | L50   | 161 | U    |
| 1   | L50   | 163 | A    |
| 1   | L50   | 164 | C    |
| 1   | L50   | 166 | A    |
| 1   | L50   | 167 | G    |
| 1   | L50   | 168 | G    |
| 1   | L50   | 169 | A    |
| 1   | L50   | 171 | U    |
| 1   | L50   | 178 | G    |
| 1   | L50   | 179 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 180 | A    |
| 1   | L50   | 184 | G    |
| 1   | L50   | 191 | A    |
| 1   | L50   | 193 | C    |
| 1   | L50   | 194 | A    |
| 1   | L50   | 199 | A    |
| 1   | L50   | 200 | C    |
| 1   | L50   | 202 | G    |
| 1   | L50   | 209 | A    |
| 1   | L50   | 210 | G    |
| 1   | L50   | 213 | U    |
| 1   | L50   | 216 | U    |
| 1   | L50   | 224 | U    |
| 1   | L50   | 225 | G    |
| 1   | L50   | 226 | A    |
| 1   | L50   | 237 | A    |
| 1   | L50   | 240 | G    |
| 1   | L50   | 243 | A    |
| 1   | L50   | 251 | U    |
| 1   | L50   | 255 | U    |
| 1   | L50   | 256 | C    |
| 1   | L50   | 266 | A    |
| 1   | L50   | 268 | C    |
| 1   | L50   | 276 | U    |
| 1   | L50   | 284 | G    |
| 1   | L50   | 285 | A    |
| 1   | L50   | 287 | A    |
| 1   | L50   | 290 | C    |
| 1   | L50   | 298 | G    |
| 1   | L50   | 302 | U    |
| 1   | L50   | 308 | A    |
| 1   | L50   | 309 | U    |
| 1   | L50   | 310 | A    |
| 1   | L50   | 311 | C    |
| 1   | L50   | 312 | G    |
| 1   | L50   | 314 | U    |
| 1   | L50   | 315 | G    |
| 1   | L50   | 316 | A    |
| 1   | L50   | 318 | U    |
| 1   | L50   | 331 | U    |
| 1   | L50   | 332 | A    |
| 1   | L50   | 333 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 340 | G    |
| 1   | L50   | 343 | A    |
| 1   | L50   | 345 | G    |
| 1   | L50   | 346 | A    |
| 1   | L50   | 347 | G    |
| 1   | L50   | 352 | C    |
| 1   | L50   | 353 | A    |
| 1   | L50   | 358 | G    |
| 1   | L50   | 360 | A    |
| 1   | L50   | 361 | U    |
| 1   | L50   | 364 | A    |
| 1   | L50   | 366 | G    |
| 1   | L50   | 371 | A    |
| 1   | L50   | 384 | A    |
| 1   | L50   | 385 | C    |
| 1   | L50   | 392 | C    |
| 1   | L50   | 396 | G    |
| 1   | L50   | 398 | A    |
| 1   | L50   | 400 | U    |
| 1   | L50   | 405 | U    |
| 1   | L50   | 408 | C    |
| 1   | L50   | 416 | A    |
| 1   | L50   | 437 | G    |
| 1   | L50   | 444 | A    |
| 1   | L50   | 449 | U    |
| 1   | L50   | 454 | C    |
| 1   | L50   | 459 | C    |
| 1   | L50   | 467 | A    |
| 1   | L50   | 481 | G    |
| 1   | L50   | 488 | C    |
| 1   | L50   | 492 | G    |
| 1   | L50   | 494 | A    |
| 1   | L50   | 495 | A    |
| 1   | L50   | 498 | U    |
| 1   | L50   | 499 | G    |
| 1   | L50   | 501 | G    |
| 1   | L50   | 503 | A    |
| 1   | L50   | 504 | G    |
| 1   | L50   | 507 | G    |
| 1   | L50   | 508 | A    |
| 1   | L50   | 509 | A    |
| 1   | L50   | 510 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 515 | U    |
| 1   | L50   | 517 | A    |
| 1   | L50   | 523 | A    |
| 1   | L50   | 524 | G    |
| 1   | L50   | 526 | G    |
| 1   | L50   | 534 | A    |
| 1   | L50   | 535 | A    |
| 1   | L50   | 537 | G    |
| 1   | L50   | 540 | G    |
| 1   | L50   | 547 | U    |
| 1   | L50   | 549 | C    |
| 1   | L50   | 556 | A    |
| 1   | L50   | 557 | U    |
| 1   | L50   | 558 | A    |
| 1   | L50   | 563 | U    |
| 1   | L50   | 564 | G    |
| 1   | L50   | 568 | A    |
| 1   | L50   | 569 | C    |
| 1   | L50   | 570 | U    |
| 1   | L50   | 580 | U    |
| 1   | L50   | 581 | G    |
| 1   | L50   | 592 | U    |
| 1   | L50   | 603 | A    |
| 1   | L50   | 604 | G    |
| 1   | L50   | 608 | G    |
| 1   | L50   | 609 | A    |
| 1   | L50   | 612 | C    |
| 1   | L50   | 615 | C    |
| 1   | L50   | 625 | U    |
| 1   | L50   | 631 | G    |
| 1   | L50   | 645 | U    |
| 1   | L50   | 647 | A    |
| 1   | L50   | 648 | G    |
| 1   | L50   | 658 | G    |
| 1   | L50   | 659 | G    |
| 1   | L50   | 665 | A    |
| 1   | L50   | 666 | A    |
| 1   | L50   | 667 | G    |
| 1   | L50   | 668 | A    |
| 1   | L50   | 672 | A    |
| 1   | L50   | 675 | G    |
| 1   | L50   | 676 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 685 | G    |
| 1   | L50   | 688 | G    |
| 1   | L50   | 695 | C    |
| 1   | L50   | 704 | A    |
| 1   | L50   | 710 | A    |
| 1   | L50   | 711 | U    |
| 1   | L50   | 716 | A    |
| 1   | L50   | 720 | C    |
| 1   | L50   | 724 | C    |
| 1   | L50   | 726 | C    |
| 1   | L50   | 727 | G    |
| 1   | L50   | 729 | A    |
| 1   | L50   | 732 | G    |
| 1   | L50   | 735 | A    |
| 1   | L50   | 736 | A    |
| 1   | L50   | 737 | G    |
| 1   | L50   | 739 | A    |
| 1   | L50   | 742 | G    |
| 1   | L50   | 749 | A    |
| 1   | L50   | 763 | U    |
| 1   | L50   | 765 | A    |
| 1   | L50   | 766 | A    |
| 1   | L50   | 767 | G    |
| 1   | L50   | 772 | C    |
| 1   | L50   | 778 | A    |
| 1   | L50   | 782 | G    |
| 1   | L50   | 795 | U    |
| 1   | L50   | 797 | U    |
| 1   | L50   | 799 | C    |
| 1   | L50   | 801 | A    |
| 1   | L50   | 802 | U    |
| 1   | L50   | 803 | G    |
| 1   | L50   | 806 | A    |
| 1   | L50   | 816 | G    |
| 1   | L50   | 830 | G    |
| 1   | L50   | 834 | G    |
| 1   | L50   | 843 | A    |
| 1   | L50   | 848 | A    |
| 1   | L50   | 849 | A    |
| 1   | L50   | 852 | A    |
| 1   | L50   | 853 | A    |
| 1   | L50   | 854 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 858 | G    |
| 1   | L50   | 859 | C    |
| 1   | L50   | 860 | A    |
| 1   | L50   | 864 | U    |
| 1   | L50   | 865 | G    |
| 1   | L50   | 867 | U    |
| 1   | L50   | 872 | A    |
| 1   | L50   | 878 | A    |
| 1   | L50   | 879 | U    |
| 1   | L50   | 881 | U    |
| 1   | L50   | 885 | G    |
| 1   | L50   | 886 | A    |
| 1   | L50   | 889 | G    |
| 1   | L50   | 893 | C    |
| 1   | L50   | 899 | G    |
| 1   | L50   | 900 | A    |
| 1   | L50   | 905 | G    |
| 1   | L50   | 915 | G    |
| 1   | L50   | 916 | A    |
| 1   | L50   | 919 | G    |
| 1   | L50   | 921 | A    |
| 1   | L50   | 922 | G    |
| 1   | L50   | 925 | C    |
| 1   | L50   | 926 | G    |
| 1   | L50   | 927 | G    |
| 1   | L50   | 930 | G    |
| 1   | L50   | 931 | C    |
| 1   | L50   | 933 | A    |
| 1   | L50   | 934 | U    |
| 1   | L50   | 935 | G    |
| 1   | L50   | 936 | G    |
| 1   | L50   | 938 | A    |
| 1   | L50   | 939 | G    |
| 1   | L50   | 940 | U    |
| 1   | L50   | 941 | C    |
| 1   | L50   | 942 | G    |
| 1   | L50   | 945 | A    |
| 1   | L50   | 946 | U    |
| 1   | L50   | 947 | C    |
| 1   | L50   | 948 | C    |
| 1   | L50   | 949 | G    |
| 1   | L50   | 950 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 951  | U    |
| 1   | L50   | 953  | A    |
| 1   | L50   | 954  | G    |
| 1   | L50   | 955  | A    |
| 1   | L50   | 956  | A    |
| 1   | L50   | 957  | A    |
| 1   | L50   | 959  | G    |
| 1   | L50   | 961  | G    |
| 1   | L50   | 963  | U    |
| 1   | L50   | 964  | A    |
| 1   | L50   | 965  | C    |
| 1   | L50   | 966  | A    |
| 1   | L50   | 967  | A    |
| 1   | L50   | 968  | C    |
| 1   | L50   | 969  | G    |
| 1   | L50   | 970  | U    |
| 1   | L50   | 971  | A    |
| 1   | L50   | 972  | C    |
| 1   | L50   | 973  | C    |
| 1   | L50   | 975  | A    |
| 1   | L50   | 978  | G    |
| 1   | L50   | 980  | A    |
| 1   | L50   | 985  | U    |
| 1   | L50   | 988  | G    |
| 1   | L50   | 993  | G    |
| 1   | L50   | 998  | U    |
| 1   | L50   | 1000 | G    |
| 1   | L50   | 1001 | A    |
| 1   | L50   | 1002 | U    |
| 1   | L50   | 1006 | G    |
| 1   | L50   | 1010 | A    |
| 1   | L50   | 1012 | C    |
| 1   | L50   | 1015 | A    |
| 1   | L50   | 1018 | U    |
| 1   | L50   | 1019 | C    |
| 1   | L50   | 1021 | G    |
| 1   | L50   | 1022 | A    |
| 1   | L50   | 1024 | G    |
| 1   | L50   | 1032 | A    |
| 1   | L50   | 1034 | C    |
| 1   | L50   | 1036 | G    |
| 1   | L50   | 1047 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1050 | U    |
| 1   | L50   | 1053 | C    |
| 1   | L50   | 1059 | G    |
| 1   | L50   | 1061 | G    |
| 1   | L50   | 1067 | A    |
| 1   | L50   | 1068 | C    |
| 1   | L50   | 1075 | A    |
| 1   | L50   | 1076 | U    |
| 1   | L50   | 1084 | G    |
| 1   | L50   | 1085 | G    |
| 1   | L50   | 1087 | G    |
| 1   | L50   | 1092 | A    |
| 1   | L50   | 1096 | A    |
| 1   | L50   | 1097 | G    |
| 1   | L50   | 1099 | G    |
| 1   | L50   | 1101 | A    |
| 1   | L50   | 1102 | G    |
| 1   | L50   | 1104 | U    |
| 1   | L50   | 1105 | C    |
| 1   | L50   | 1111 | G    |
| 1   | L50   | 1116 | U    |
| 1   | L50   | 1117 | A    |
| 1   | L50   | 1120 | G    |
| 1   | L50   | 1121 | A    |
| 1   | L50   | 1123 | A    |
| 1   | L50   | 1124 | A    |
| 1   | L50   | 1130 | C    |
| 1   | L50   | 1131 | U    |
| 1   | L50   | 1133 | C    |
| 1   | L50   | 1135 | G    |
| 1   | L50   | 1136 | C    |
| 1   | L50   | 1140 | A    |
| 1   | L50   | 1141 | A    |
| 1   | L50   | 1142 | A    |
| 1   | L50   | 1144 | A    |
| 1   | L50   | 1148 | A    |
| 1   | L50   | 1149 | G    |
| 1   | L50   | 1150 | G    |
| 1   | L50   | 1155 | G    |
| 1   | L50   | 1163 | U    |
| 1   | L50   | 1169 | C    |
| 1   | L50   | 1170 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1171 | U    |
| 1   | L50   | 1172 | A    |
| 1   | L50   | 1173 | A    |
| 1   | L50   | 1176 | A    |
| 1   | L50   | 1177 | G    |
| 1   | L50   | 1181 | G    |
| 1   | L50   | 1182 | A    |
| 1   | L50   | 1183 | G    |
| 1   | L50   | 1185 | C    |
| 1   | L50   | 1189 | U    |
| 1   | L50   | 1192 | A    |
| 1   | L50   | 1198 | G    |
| 1   | L50   | 1204 | A    |
| 1   | L50   | 1206 | A    |
| 1   | L50   | 1217 | A    |
| 1   | L50   | 1218 | A    |
| 1   | L50   | 1223 | A    |
| 1   | L50   | 1226 | C    |
| 1   | L50   | 1227 | A    |
| 1   | L50   | 1229 | G    |
| 1   | L50   | 1231 | U    |
| 1   | L50   | 1232 | G    |
| 1   | L50   | 1233 | A    |
| 1   | L50   | 1235 | A    |
| 1   | L50   | 1236 | U    |
| 1   | L50   | 1237 | U    |
| 1   | L50   | 1247 | G    |
| 1   | L50   | 1250 | C    |
| 1   | L50   | 1254 | C    |
| 1   | L50   | 1257 | A    |
| 1   | L50   | 1264 | C    |
| 1   | L50   | 1268 | U    |
| 1   | L50   | 1270 | U    |
| 1   | L50   | 1271 | U    |
| 1   | L50   | 1273 | G    |
| 1   | L50   | 1274 | C    |
| 1   | L50   | 1278 | U    |
| 1   | L50   | 1281 | A    |
| 1   | L50   | 1283 | A    |
| 1   | L50   | 1308 | A    |
| 1   | L50   | 1309 | C    |
| 1   | L50   | 1318 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1327 | A    |
| 1   | L50   | 1332 | G    |
| 1   | L50   | 1339 | G    |
| 1   | L50   | 1340 | A    |
| 1   | L50   | 1341 | G    |
| 1   | L50   | 1342 | A    |
| 1   | L50   | 1346 | A    |
| 1   | L50   | 1351 | C    |
| 1   | L50   | 1360 | U    |
| 1   | L50   | 1374 | U    |
| 1   | L50   | 1375 | G    |
| 1   | L50   | 1383 | C    |
| 1   | L50   | 1385 | G    |
| 1   | L50   | 1387 | G    |
| 1   | L50   | 1388 | C    |
| 1   | L50   | 1391 | G    |
| 1   | L50   | 1393 | U    |
| 1   | L50   | 1395 | U    |
| 1   | L50   | 1396 | G    |
| 1   | L50   | 1400 | A    |
| 1   | L50   | 1411 | C    |
| 1   | L50   | 1412 | C    |
| 1   | L50   | 1414 | U    |
| 1   | L50   | 1415 | G    |
| 1   | L50   | 1416 | A    |
| 1   | L50   | 1417 | A    |
| 1   | L50   | 1421 | A    |
| 1   | L50   | 1427 | A    |
| 1   | L50   | 1429 | A    |
| 1   | L50   | 1430 | U    |
| 1   | L50   | 1431 | G    |
| 1   | L50   | 1437 | A    |
| 1   | L50   | 1441 | U    |
| 1   | L50   | 1449 | A    |
| 1   | L50   | 1450 | A    |
| 1   | L50   | 1454 | U    |
| 1   | L50   | 1457 | C    |
| 1   | L50   | 1458 | A    |
| 1   | L50   | 1463 | U    |
| 1   | L50   | 1465 | C    |
| 1   | L50   | 1466 | A    |
| 1   | L50   | 1468 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1474 | G    |
| 1   | L50   | 1485 | G    |
| 1   | L50   | 1486 | G    |
| 1   | L50   | 1488 | U    |
| 1   | L50   | 1489 | G    |
| 1   | L50   | 1490 | U    |
| 1   | L50   | 1491 | U    |
| 1   | L50   | 1492 | U    |
| 1   | L50   | 1499 | U    |
| 1   | L50   | 1500 | G    |
| 1   | L50   | 1503 | A    |
| 1   | L50   | 1504 | G    |
| 1   | L50   | 1506 | G    |
| 1   | L50   | 1513 | G    |
| 1   | L50   | 1527 | U    |
| 1   | L50   | 1535 | G    |
| 1   | L50   | 1536 | G    |
| 1   | L50   | 1539 | A    |
| 1   | L50   | 1547 | G    |
| 1   | L50   | 1554 | U    |
| 1   | L50   | 1555 | G    |
| 1   | L50   | 1556 | U    |
| 1   | L50   | 1557 | G    |
| 1   | L50   | 1563 | A    |
| 1   | L50   | 1564 | U    |
| 1   | L50   | 1565 | U    |
| 1   | L50   | 1571 | A    |
| 1   | L50   | 1573 | G    |
| 1   | L50   | 1574 | G    |
| 1   | L50   | 1583 | A    |
| 1   | L50   | 1592 | U    |
| 1   | L50   | 1603 | C    |
| 1   | L50   | 1609 | G    |
| 1   | L50   | 1610 | A    |
| 1   | L50   | 1611 | A    |
| 1   | L50   | 1612 | G    |
| 1   | L50   | 1613 | A    |
| 1   | L50   | 1614 | G    |
| 1   | L50   | 1619 | G    |
| 1   | L50   | 1625 | A    |
| 1   | L50   | 1626 | G    |
| 1   | L50   | 1628 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1629 | C    |
| 1   | L50   | 1643 | G    |
| 1   | L50   | 1645 | C    |
| 1   | L50   | 1649 | A    |
| 1   | L50   | 1651 | A    |
| 1   | L50   | 1653 | G    |
| 1   | L50   | 1668 | A    |
| 1   | L50   | 1675 | G    |
| 1   | L50   | 1679 | A    |
| 1   | L50   | 1680 | A    |
| 1   | L50   | 1685 | G    |
| 1   | L50   | 1687 | G    |
| 1   | L50   | 1688 | A    |
| 1   | L50   | 1692 | A    |
| 1   | L50   | 1693 | C    |
| 1   | L50   | 1700 | U    |
| 1   | L50   | 1705 | U    |
| 1   | L50   | 1706 | A    |
| 1   | L50   | 1708 | G    |
| 1   | L50   | 1709 | G    |
| 1   | L50   | 1715 | A    |
| 1   | L50   | 1717 | A    |
| 1   | L50   | 1718 | C    |
| 1   | L50   | 1720 | C    |
| 1   | L50   | 1723 | C    |
| 1   | L50   | 1724 | G    |
| 1   | L50   | 1731 | A    |
| 1   | L50   | 1733 | A    |
| 1   | L50   | 1734 | U    |
| 1   | L50   | 1739 | A    |
| 1   | L50   | 1740 | C    |
| 1   | L50   | 1742 | C    |
| 1   | L50   | 1743 | G    |
| 1   | L50   | 1744 | C    |
| 1   | L50   | 1746 | U    |
| 1   | L50   | 1749 | A    |
| 1   | L50   | 1751 | G    |
| 1   | L50   | 1753 | A    |
| 1   | L50   | 1754 | A    |
| 1   | L50   | 1755 | U    |
| 1   | L50   | 1756 | G    |
| 1   | L50   | 1760 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1771 | G    |
| 1   | L50   | 1772 | U    |
| 1   | L50   | 1797 | A    |
| 1   | L50   | 1801 | C    |
| 1   | L50   | 1803 | A    |
| 1   | L50   | 1808 | A    |
| 1   | L50   | 1809 | A    |
| 1   | L50   | 1810 | C    |
| 1   | L50   | 1811 | G    |
| 1   | L50   | 1828 | G    |
| 1   | L50   | 1832 | A    |
| 1   | L50   | 1836 | A    |
| 1   | L50   | 1837 | A    |
| 1   | L50   | 1838 | G    |
| 1   | L50   | 1839 | A    |
| 1   | L50   | 1846 | U    |
| 1   | L50   | 1854 | A    |
| 1   | L50   | 1862 | G    |
| 1   | L50   | 1869 | A    |
| 1   | L50   | 1876 | A    |
| 1   | L50   | 1880 | U    |
| 1   | L50   | 1882 | G    |
| 1   | L50   | 1883 | A    |
| 1   | L50   | 1884 | G    |
| 1   | L50   | 1885 | G    |
| 1   | L50   | 1886 | C    |
| 1   | L50   | 1887 | G    |
| 1   | L50   | 1889 | U    |
| 1   | L50   | 1890 | G    |
| 1   | L50   | 1893 | G    |
| 1   | L50   | 1895 | A    |
| 1   | L50   | 1896 | A    |
| 1   | L50   | 1897 | G    |
| 1   | L50   | 1898 | G    |
| 1   | L50   | 1899 | U    |
| 1   | L50   | 1902 | A    |
| 1   | L50   | 1903 | G    |
| 1   | L50   | 1905 | G    |
| 1   | L50   | 1912 | C    |
| 1   | L50   | 1915 | A    |
| 1   | L50   | 1916 | A    |
| 1   | L50   | 1917 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1919 | G    |
| 1   | L50   | 1920 | A    |
| 1   | L50   | 1921 | A    |
| 1   | L50   | 1923 | G    |
| 1   | L50   | 1927 | A    |
| 1   | L50   | 1928 | C    |
| 1   | L50   | 1929 | U    |
| 1   | L50   | 1930 | G    |
| 1   | L50   | 1931 | C    |
| 1   | L50   | 1933 | C    |
| 1   | L50   | 1934 | C    |
| 1   | L50   | 1937 | G    |
| 1   | L50   | 1939 | U    |
| 1   | L50   | 1940 | C    |
| 1   | L50   | 1947 | A    |
| 1   | L50   | 1950 | C    |
| 1   | L50   | 1951 | A    |
| 1   | L50   | 1953 | U    |
| 1   | L50   | 1956 | U    |
| 1   | L50   | 1957 | U    |
| 1   | L50   | 1958 | U    |
| 1   | L50   | 1959 | A    |
| 1   | L50   | 1961 | G    |
| 1   | L50   | 1962 | G    |
| 1   | L50   | 1963 | A    |
| 1   | L50   | 1964 | C    |
| 1   | L50   | 1967 | A    |
| 1   | L50   | 1977 | G    |
| 1   | L50   | 1978 | G    |
| 1   | L50   | 1983 | U    |
| 1   | L50   | 1985 | G    |
| 1   | L50   | 1990 | G    |
| 1   | L50   | 1991 | G    |
| 1   | L50   | 1995 | G    |
| 1   | L50   | 1997 | A    |
| 1   | L50   | 1999 | G    |
| 1   | L50   | 2008 | A    |
| 1   | L50   | 2011 | A    |
| 1   | L50   | 2013 | A    |
| 1   | L50   | 2019 | G    |
| 1   | L50   | 2023 | A    |
| 1   | L50   | 2027 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2028 | A    |
| 1   | L50   | 2036 | A    |
| 1   | L50   | 2037 | C    |
| 1   | L50   | 2039 | G    |
| 1   | L50   | 2042 | A    |
| 1   | L50   | 2043 | G    |
| 1   | L50   | 2044 | A    |
| 1   | L50   | 2045 | C    |
| 1   | L50   | 2046 | G    |
| 1   | L50   | 2047 | A    |
| 1   | L50   | 2048 | G    |
| 1   | L50   | 2053 | C    |
| 1   | L50   | 2054 | U    |
| 1   | L50   | 2055 | C    |
| 1   | L50   | 2057 | U    |
| 1   | L50   | 2059 | U    |
| 1   | L50   | 2060 | A    |
| 1   | L50   | 2061 | G    |
| 1   | L50   | 2062 | A    |
| 1   | L50   | 2067 | A    |
| 1   | L50   | 2073 | U    |
| 1   | L50   | 2075 | A    |
| 1   | L50   | 2076 | A    |
| 1   | L50   | 2077 | G    |
| 1   | L50   | 2078 | A    |
| 1   | L50   | 2079 | G    |
| 1   | L50   | 2085 | G    |
| 1   | L50   | 2087 | G    |
| 1   | L50   | 2093 | G    |
| 1   | L50   | 2098 | A    |
| 1   | L50   | 2109 | G    |
| 1   | L50   | 2110 | A    |
| 1   | L50   | 2111 | G    |
| 1   | L50   | 2122 | G    |
| 1   | L50   | 2124 | C    |
| 1   | L50   | 2130 | G    |
| 1   | L50   | 2131 | A    |
| 1   | L50   | 2136 | A    |
| 1   | L50   | 2140 | A    |
| 1   | L50   | 2141 | U    |
| 1   | L50   | 2142 | A    |
| 1   | L50   | 2145 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2152 | U    |
| 1   | L50   | 2159 | U    |
| 1   | L50   | 2164 | G    |
| 1   | L50   | 2168 | G    |
| 1   | L50   | 2169 | A    |
| 1   | L50   | 2170 | A    |
| 1   | L50   | 2178 | C    |
| 1   | L50   | 2184 | G    |
| 1   | L50   | 2185 | A    |
| 1   | L50   | 2206 | A    |
| 1   | L50   | 2210 | U    |
| 1   | L50   | 2211 | A    |
| 1   | L50   | 2213 | A    |
| 1   | L50   | 2218 | G    |
| 1   | L50   | 2221 | G    |
| 1   | L50   | 2227 | U    |
| 1   | L50   | 2228 | U    |
| 1   | L50   | 2229 | U    |
| 1   | L50   | 2235 | C    |
| 1   | L50   | 2239 | G    |
| 1   | L50   | 2243 | U    |
| 1   | L50   | 2253 | C    |
| 1   | L50   | 2255 | A    |
| 1   | L50   | 2260 | G    |
| 1   | L50   | 2262 | C    |
| 1   | L50   | 2266 | G    |
| 1   | L50   | 2267 | C    |
| 1   | L50   | 2268 | A    |
| 1   | L50   | 2269 | G    |
| 1   | L50   | 2270 | C    |
| 1   | L50   | 2272 | G    |
| 1   | L50   | 2279 | A    |
| 1   | L50   | 2282 | G    |
| 1   | L50   | 2291 | U    |
| 1   | L50   | 2296 | C    |
| 1   | L50   | 2303 | C    |
| 1   | L50   | 2304 | A    |
| 1   | L50   | 2309 | A    |
| 1   | L50   | 2310 | C    |
| 1   | L50   | 2313 | G    |
| 1   | L50   | 2319 | G    |
| 1   | L50   | 2322 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2323 | U    |
| 1   | L50   | 2325 | G    |
| 1   | L50   | 2335 | A    |
| 1   | L50   | 2339 | A    |
| 1   | L50   | 2340 | G    |
| 1   | L50   | 2345 | G    |
| 1   | L50   | 2351 | U    |
| 1   | L50   | 2355 | A    |
| 1   | L50   | 2360 | C    |
| 1   | L50   | 2366 | A    |
| 1   | L50   | 2368 | U    |
| 1   | L50   | 2376 | A    |
| 1   | L50   | 2377 | G    |
| 1   | L50   | 2379 | G    |
| 1   | L50   | 2388 | U    |
| 1   | L50   | 2391 | G    |
| 1   | L50   | 2401 | C    |
| 1   | L50   | 2420 | C    |
| 1   | L50   | 2423 | C    |
| 1   | L50   | 2428 | G    |
| 1   | L50   | 2435 | A    |
| 1   | L50   | 2436 | G    |
| 1   | L50   | 2441 | A    |
| 1   | L50   | 2447 | A    |
| 1   | L50   | 2453 | C    |
| 1   | L50   | 2454 | G    |
| 1   | L50   | 2458 | C    |
| 1   | L50   | 2459 | C    |
| 1   | L50   | 2460 | U    |
| 1   | L50   | 2467 | U    |
| 1   | L50   | 2469 | G    |
| 1   | L50   | 2470 | C    |
| 1   | L50   | 2471 | U    |
| 1   | L50   | 2473 | G    |
| 1   | L50   | 2474 | A    |
| 1   | L50   | 2477 | C    |
| 1   | L50   | 2478 | C    |
| 1   | L50   | 2480 | C    |
| 1   | L50   | 2481 | U    |
| 1   | L50   | 2482 | A    |
| 1   | L50   | 2483 | A    |
| 1   | L50   | 2487 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2488 | G    |
| 1   | L50   | 2490 | A    |
| 1   | L50   | 2491 | A    |
| 1   | L50   | 2501 | A    |
| 1   | L50   | 2519 | G    |
| 1   | L50   | 2520 | A    |
| 1   | L50   | 2534 | U    |
| 1   | L50   | 2535 | U    |
| 1   | L50   | 2539 | A    |
| 1   | L50   | 2540 | G    |
| 1   | L50   | 2542 | G    |
| 1   | L50   | 2543 | G    |
| 1   | L50   | 2549 | U    |
| 1   | L50   | 2553 | A    |
| 1   | L50   | 2561 | U    |
| 1   | L50   | 2562 | U    |
| 1   | L50   | 2563 | U    |
| 1   | L50   | 2568 | U    |
| 1   | L50   | 2582 | G    |
| 1   | L50   | 2588 | G    |
| 1   | L50   | 2595 | U    |
| 1   | L50   | 2596 | G    |
| 1   | L50   | 2598 | U    |
| 1   | L50   | 2599 | U    |
| 1   | L50   | 2606 | A    |
| 2   | S60   | 2    | C    |
| 2   | S60   | 3    | C    |
| 2   | S60   | 7    | U    |
| 2   | S60   | 8    | U    |
| 2   | S60   | 18   | U    |
| 2   | S60   | 32   | G    |
| 2   | S60   | 33   | U    |
| 2   | S60   | 35   | U    |
| 2   | S60   | 39   | A    |
| 2   | S60   | 40   | G    |
| 2   | S60   | 41   | A    |
| 2   | S60   | 43   | U    |
| 2   | S60   | 45   | A    |
| 2   | S60   | 48   | C    |
| 2   | S60   | 54   | U    |
| 2   | S60   | 55   | G    |
| 2   | S60   | 56   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S60   | 57  | G    |
| 2   | S60   | 58  | U    |
| 2   | S60   | 59  | A    |
| 2   | S60   | 61  | G    |
| 2   | S60   | 62  | C    |
| 2   | S60   | 63  | G    |
| 2   | S60   | 64  | A    |
| 2   | S60   | 65  | A    |
| 2   | S60   | 66  | G    |
| 2   | S60   | 68  | G    |
| 2   | S60   | 69  | A    |
| 2   | S60   | 71  | U    |
| 2   | S60   | 72  | A    |
| 2   | S60   | 74  | U    |
| 2   | S60   | 75  | G    |
| 2   | S60   | 76  | A    |
| 2   | S60   | 77  | A    |
| 2   | S60   | 78  | G    |
| 2   | S60   | 79  | C    |
| 2   | S60   | 80  | G    |
| 2   | S60   | 84  | G    |
| 2   | S60   | 85  | A    |
| 2   | S60   | 86  | A    |
| 2   | S60   | 92  | A    |
| 2   | S60   | 94  | U    |
| 2   | S60   | 96  | A    |
| 2   | S60   | 97  | C    |
| 2   | S60   | 106 | A    |
| 2   | S60   | 107 | U    |
| 2   | S60   | 116 | U    |
| 2   | S60   | 118 | G    |
| 2   | S60   | 119 | A    |
| 2   | S60   | 121 | C    |
| 2   | S60   | 127 | A    |
| 2   | S60   | 128 | A    |
| 2   | S60   | 130 | C    |
| 2   | S60   | 133 | A    |
| 2   | S60   | 134 | G    |
| 2   | S60   | 135 | G    |
| 2   | S60   | 136 | A    |
| 2   | S60   | 137 | A    |
| 2   | S60   | 138 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S60   | 140 | A    |
| 2   | S60   | 141 | G    |
| 2   | S60   | 142 | A    |
| 2   | S60   | 143 | G    |
| 2   | S60   | 144 | G    |
| 2   | S60   | 149 | A    |
| 2   | S60   | 150 | A    |
| 2   | S60   | 181 | A    |
| 2   | S60   | 183 | G    |
| 2   | S60   | 184 | A    |
| 2   | S60   | 186 | A    |
| 2   | S60   | 187 | A    |
| 2   | S60   | 188 | C    |
| 2   | S60   | 190 | A    |
| 2   | S60   | 191 | C    |
| 2   | S60   | 193 | G    |
| 2   | S60   | 194 | U    |
| 2   | S60   | 195 | G    |
| 2   | S60   | 197 | A    |
| 2   | S60   | 204 | U    |
| 2   | S60   | 205 | A    |
| 2   | S60   | 214 | U    |
| 2   | S60   | 215 | C    |
| 2   | S60   | 220 | C    |
| 2   | S60   | 221 | A    |
| 2   | S60   | 222 | G    |
| 2   | S60   | 226 | G    |
| 2   | S60   | 241 | G    |
| 2   | S60   | 242 | C    |
| 2   | S60   | 247 | U    |
| 2   | S60   | 255 | A    |
| 2   | S60   | 256 | G    |
| 2   | S60   | 263 | A    |
| 2   | S60   | 264 | C    |
| 2   | S60   | 266 | G    |
| 2   | S60   | 268 | G    |
| 2   | S60   | 280 | G    |
| 2   | S60   | 281 | A    |
| 2   | S60   | 283 | U    |
| 2   | S60   | 284 | C    |
| 2   | S60   | 287 | G    |
| 2   | S60   | 288 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S60   | 289 | G    |
| 2   | S60   | 302 | A    |
| 2   | S60   | 303 | G    |
| 2   | S60   | 304 | A    |
| 2   | S60   | 305 | C    |
| 2   | S60   | 306 | G    |
| 2   | S60   | 307 | G    |
| 2   | S60   | 309 | U    |
| 2   | S60   | 310 | A    |
| 2   | S60   | 311 | C    |
| 2   | S60   | 315 | G    |
| 2   | S60   | 317 | C    |
| 2   | S60   | 318 | C    |
| 2   | S60   | 319 | A    |
| 2   | S60   | 320 | A    |
| 2   | S60   | 321 | G    |
| 2   | S60   | 327 | C    |
| 2   | S60   | 328 | A    |
| 2   | S60   | 329 | G    |
| 2   | S60   | 331 | A    |
| 2   | S60   | 337 | G    |
| 2   | S60   | 339 | A    |
| 2   | S60   | 340 | A    |
| 2   | S60   | 341 | A    |
| 2   | S60   | 342 | U    |
| 2   | S60   | 343 | U    |
| 2   | S60   | 347 | G    |
| 2   | S60   | 355 | C    |
| 2   | S60   | 356 | A    |
| 2   | S60   | 357 | A    |
| 2   | S60   | 358 | G    |
| 2   | S60   | 362 | G    |
| 2   | S60   | 363 | C    |
| 2   | S60   | 364 | G    |
| 2   | S60   | 371 | A    |
| 2   | S60   | 372 | A    |
| 2   | S60   | 378 | G    |
| 2   | S60   | 380 | G    |
| 2   | S60   | 383 | A    |
| 2   | S60   | 384 | A    |
| 2   | S60   | 385 | C    |
| 2   | S60   | 387 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S60   | 388 | G    |
| 2   | S60   | 389 | U    |
| 2   | S60   | 390 | G    |
| 2   | S60   | 391 | U    |
| 2   | S60   | 392 | G    |
| 2   | S60   | 393 | U    |
| 2   | S60   | 394 | G    |
| 2   | S60   | 398 | A    |
| 2   | S60   | 400 | A    |
| 2   | S60   | 401 | C    |
| 2   | S60   | 403 | A    |
| 2   | S60   | 404 | C    |
| 2   | S60   | 406 | U    |
| 2   | S60   | 407 | G    |
| 2   | S60   | 408 | A    |
| 2   | S60   | 409 | G    |
| 2   | S60   | 414 | U    |
| 2   | S60   | 416 | G    |
| 2   | S60   | 418 | G    |
| 2   | S60   | 420 | U    |
| 2   | S60   | 421 | C    |
| 2   | S60   | 422 | A    |
| 2   | S60   | 424 | G    |
| 2   | S60   | 425 | G    |
| 2   | S60   | 426 | C    |
| 2   | S60   | 429 | G    |
| 2   | S60   | 430 | U    |
| 2   | S60   | 431 | G    |
| 2   | S60   | 432 | C    |
| 2   | S60   | 434 | A    |
| 2   | S60   | 435 | G    |
| 2   | S60   | 437 | A    |
| 2   | S60   | 438 | U    |
| 2   | S60   | 439 | C    |
| 2   | S60   | 440 | C    |
| 2   | S60   | 441 | G    |
| 2   | S60   | 443 | G    |
| 2   | S60   | 444 | G    |
| 2   | S60   | 445 | U    |
| 2   | S60   | 446 | A    |
| 2   | S60   | 447 | A    |
| 2   | S60   | 448 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S60   | 449 | A    |
| 2   | S60   | 450 | C    |
| 2   | S60   | 451 | C    |
| 2   | S60   | 452 | A    |
| 2   | S60   | 453 | G    |
| 2   | S60   | 461 | A    |
| 2   | S60   | 462 | G    |
| 2   | S60   | 463 | U    |
| 2   | S60   | 465 | U    |
| 2   | S60   | 468 | A    |
| 2   | S60   | 474 | A    |
| 2   | S60   | 477 | G    |
| 2   | S60   | 478 | C    |
| 2   | S60   | 484 | U    |
| 2   | S60   | 486 | A    |
| 2   | S60   | 487 | A    |
| 2   | S60   | 490 | G    |
| 2   | S60   | 499 | U    |
| 2   | S60   | 501 | G    |
| 2   | S60   | 502 | A    |
| 2   | S60   | 505 | A    |
| 2   | S60   | 506 | A    |
| 2   | S60   | 507 | C    |
| 2   | S60   | 510 | U    |
| 2   | S60   | 512 | C    |
| 2   | S60   | 520 | U    |
| 2   | S60   | 521 | A    |
| 2   | S60   | 523 | U    |
| 2   | S60   | 524 | G    |
| 2   | S60   | 527 | G    |
| 2   | S60   | 535 | A    |
| 2   | S60   | 540 | C    |
| 2   | S60   | 554 | A    |
| 2   | S60   | 562 | G    |
| 2   | S60   | 565 | U    |
| 2   | S60   | 566 | A    |
| 2   | S60   | 567 | A    |
| 2   | S60   | 568 | G    |
| 2   | S60   | 570 | A    |
| 2   | S60   | 578 | A    |
| 2   | S60   | 581 | G    |
| 2   | S60   | 582 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S60   | 587 | U    |
| 2   | S60   | 590 | U    |
| 2   | S60   | 593 | A    |
| 2   | S60   | 599 | G    |
| 2   | S60   | 600 | A    |
| 2   | S60   | 601 | G    |
| 2   | S60   | 608 | A    |
| 2   | S60   | 609 | A    |
| 2   | S60   | 610 | U    |
| 2   | S60   | 621 | G    |
| 2   | S60   | 622 | C    |
| 2   | S60   | 623 | U    |
| 2   | S60   | 624 | U    |
| 2   | S60   | 627 | G    |
| 2   | S60   | 635 | G    |
| 2   | S60   | 646 | G    |
| 2   | S60   | 647 | C    |
| 2   | S60   | 653 | A    |
| 2   | S60   | 662 | U    |
| 2   | S60   | 668 | G    |
| 2   | S60   | 676 | A    |
| 2   | S60   | 680 | A    |
| 2   | S60   | 685 | G    |
| 2   | S60   | 686 | G    |
| 2   | S60   | 687 | A    |
| 2   | S60   | 690 | A    |
| 2   | S60   | 694 | A    |
| 2   | S60   | 700 | A    |
| 2   | S60   | 702 | U    |
| 2   | S60   | 703 | A    |
| 2   | S60   | 705 | A    |
| 2   | S60   | 707 | A    |
| 2   | S60   | 712 | A    |
| 2   | S60   | 714 | U    |
| 2   | S60   | 716 | G    |
| 2   | S60   | 722 | G    |
| 2   | S60   | 728 | A    |
| 2   | S60   | 730 | C    |
| 2   | S60   | 731 | G    |
| 2   | S60   | 732 | A    |
| 2   | S60   | 733 | U    |
| 2   | S60   | 734 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S60   | 736 | C    |
| 2   | S60   | 738 | A    |
| 2   | S60   | 739 | C    |
| 2   | S60   | 740 | G    |
| 2   | S60   | 749 | G    |
| 2   | S60   | 752 | A    |
| 2   | S60   | 754 | G    |
| 2   | S60   | 755 | A    |
| 2   | S60   | 756 | G    |
| 2   | S60   | 760 | G    |
| 2   | S60   | 768 | A    |
| 2   | S60   | 775 | U    |
| 2   | S60   | 776 | A    |
| 2   | S60   | 777 | G    |
| 2   | S60   | 778 | U    |
| 2   | S60   | 780 | G    |
| 2   | S60   | 781 | G    |
| 2   | S60   | 788 | G    |
| 2   | S60   | 806 | G    |
| 2   | S60   | 808 | G    |
| 2   | S60   | 812 | A    |
| 2   | S60   | 817 | A    |
| 2   | S60   | 818 | A    |
| 2   | S60   | 820 | G    |
| 2   | S60   | 824 | A    |
| 2   | S60   | 826 | U    |
| 2   | S60   | 828 | A    |
| 2   | S60   | 830 | G    |
| 2   | S60   | 831 | G    |
| 2   | S60   | 832 | A    |
| 2   | S60   | 833 | A    |
| 2   | S60   | 835 | A    |
| 2   | S60   | 836 | A    |
| 2   | S60   | 839 | C    |
| 2   | S60   | 840 | C    |
| 2   | S60   | 841 | A    |
| 2   | S60   | 849 | U    |
| 2   | S60   | 852 | A    |
| 2   | S60   | 854 | U    |
| 2   | S60   | 866 | U    |
| 2   | S60   | 868 | U    |
| 2   | S60   | 872 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S60   | 873 | C    |
| 2   | S60   | 874 | A    |
| 2   | S60   | 875 | A    |
| 2   | S60   | 877 | G    |
| 2   | S60   | 878 | C    |
| 2   | S60   | 879 | G    |
| 2   | S60   | 880 | G    |
| 2   | S60   | 883 | C    |
| 2   | S60   | 884 | A    |
| 2   | S60   | 887 | U    |
| 2   | S60   | 890 | C    |
| 2   | S60   | 898 | G    |
| 2   | S60   | 899 | A    |
| 2   | S60   | 906 | U    |
| 2   | S60   | 908 | U    |
| 2   | S60   | 909 | G    |
| 2   | S60   | 911 | G    |
| 2   | S60   | 912 | C    |
| 2   | S60   | 913 | G    |
| 2   | S60   | 914 | U    |
| 2   | S60   | 915 | A    |
| 2   | S60   | 916 | G    |
| 2   | S60   | 917 | U    |
| 2   | S60   | 918 | A    |
| 2   | S60   | 919 | C    |
| 2   | S60   | 921 | C    |
| 2   | S60   | 922 | G    |
| 2   | S60   | 924 | U    |
| 2   | S60   | 925 | A    |
| 2   | S60   | 926 | G    |
| 2   | S60   | 927 | G    |
| 2   | S60   | 929 | C    |
| 2   | S60   | 937 | G    |
| 2   | S60   | 941 | C    |
| 2   | S60   | 947 | C    |
| 2   | S60   | 948 | G    |
| 2   | S60   | 950 | U    |
| 2   | S60   | 952 | A    |
| 2   | S60   | 953 | C    |
| 2   | S60   | 955 | A    |
| 2   | S60   | 957 | G    |
| 2   | S60   | 959 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S60   | 960  | U    |
| 2   | S60   | 968  | C    |
| 2   | S60   | 969  | C    |
| 2   | S60   | 970  | U    |
| 2   | S60   | 971  | U    |
| 2   | S60   | 972  | U    |
| 2   | S60   | 974  | G    |
| 2   | S60   | 980  | G    |
| 2   | S60   | 981  | U    |
| 2   | S60   | 985  | C    |
| 2   | S60   | 986  | G    |
| 2   | S60   | 987  | A    |
| 2   | S60   | 988  | A    |
| 2   | S60   | 989  | G    |
| 2   | S60   | 990  | U    |
| 2   | S60   | 992  | G    |
| 2   | S60   | 995  | A    |
| 2   | S60   | 996  | G    |
| 2   | S60   | 998  | U    |
| 2   | S60   | 1000 | C    |
| 2   | S60   | 1001 | C    |
| 2   | S60   | 1003 | A    |
| 2   | S60   | 1004 | G    |
| 2   | S60   | 1005 | G    |
| 2   | S60   | 1006 | A    |
| 2   | S60   | 1011 | A    |
| 2   | S60   | 1012 | A    |
| 2   | S60   | 1013 | A    |
| 2   | S60   | 1014 | G    |
| 2   | S60   | 1017 | A    |
| 2   | S60   | 1018 | U    |
| 2   | S60   | 1019 | C    |
| 2   | S60   | 1021 | A    |
| 2   | S60   | 1022 | C    |
| 2   | S60   | 1023 | A    |
| 2   | S60   | 1024 | G    |
| 2   | S60   | 1028 | U    |
| 2   | S60   | 1029 | U    |
| 2   | S60   | 1030 | A    |
| 2   | S60   | 1031 | A    |
| 2   | S60   | 1033 | A    |
| 2   | S60   | 1034 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S60   | 1037 | C    |
| 2   | S60   | 1039 | G    |
| 2   | S60   | 1040 | G    |
| 2   | S60   | 1041 | A    |
| 2   | S60   | 1042 | A    |
| 2   | S60   | 1043 | G    |
| 2   | S60   | 1044 | G    |
| 2   | S60   | 1045 | A    |
| 2   | S60   | 1046 | A    |
| 2   | S60   | 1047 | G    |
| 2   | S60   | 1048 | G    |
| 2   | S60   | 1049 | G    |
| 2   | S60   | 1050 | G    |
| 2   | S60   | 1051 | C    |
| 2   | S60   | 1052 | A    |
| 2   | S60   | 1053 | A    |
| 2   | S60   | 1055 | A    |
| 2   | S60   | 1056 | A    |
| 2   | S60   | 1057 | C    |
| 2   | S60   | 1058 | A    |
| 2   | S60   | 1059 | G    |
| 2   | S60   | 1060 | G    |
| 2   | S60   | 1061 | U    |
| 2   | S60   | 1062 | C    |
| 2   | S60   | 1063 | A    |
| 2   | S60   | 1064 | G    |
| 2   | S60   | 1065 | U    |
| 2   | S60   | 1066 | G    |
| 2   | S60   | 1067 | A    |
| 2   | S60   | 1071 | C    |
| 2   | S60   | 1073 | U    |
| 2   | S60   | 1075 | A    |
| 2   | S60   | 1076 | G    |
| 2   | S60   | 1077 | A    |
| 2   | S60   | 1083 | U    |
| 2   | S60   | 1084 | G    |
| 2   | S60   | 1085 | G    |
| 2   | S60   | 1089 | G    |
| 2   | S60   | 1090 | C    |
| 2   | S60   | 1091 | A    |
| 2   | S60   | 1094 | C    |
| 2   | S60   | 1096 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S60   | 1097 | A    |
| 2   | S60   | 1100 | A    |
| 2   | S60   | 1102 | A    |
| 2   | S60   | 1103 | G    |
| 2   | S60   | 1105 | G    |
| 2   | S60   | 1110 | C    |
| 2   | S60   | 1113 | C    |
| 2   | S60   | 1114 | A    |
| 2   | S60   | 1116 | A    |
| 2   | S60   | 1117 | A    |
| 2   | S60   | 1118 | A    |
| 2   | S60   | 1119 | C    |
| 2   | S60   | 1120 | A    |
| 2   | S60   | 1121 | A    |
| 2   | S60   | 1122 | A    |
| 2   | S60   | 1123 | U    |
| 2   | S60   | 1124 | A    |
| 2   | S60   | 1125 | G    |
| 2   | S60   | 1126 | A    |
| 2   | S60   | 1127 | A    |
| 2   | S60   | 1130 | A    |
| 2   | S60   | 1132 | A    |
| 2   | S60   | 1133 | U    |
| 2   | S60   | 1136 | G    |
| 2   | S60   | 1137 | A    |
| 2   | S60   | 1138 | U    |
| 2   | S60   | 1139 | C    |
| 2   | S60   | 1141 | A    |
| 2   | S60   | 1142 | G    |
| 2   | S60   | 1143 | A    |
| 2   | S60   | 1146 | G    |
| 2   | S60   | 1155 | C    |
| 2   | S60   | 1158 | U    |
| 2   | S60   | 1161 | U    |
| 2   | S60   | 1164 | G    |
| 2   | S60   | 1165 | C    |
| 2   | S60   | 1166 | A    |
| 2   | S60   | 1168 | A    |
| 2   | S60   | 1169 | G    |
| 2   | S60   | 1171 | A    |
| 2   | S60   | 1173 | C    |
| 2   | S60   | 1178 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S60   | 1182 | G    |
| 2   | S60   | 1185 | A    |
| 2   | S60   | 1190 | U    |
| 2   | S60   | 1191 | C    |
| 2   | S60   | 1192 | G    |
| 2   | S60   | 1193 | U    |
| 2   | S60   | 1195 | A    |
| 2   | S60   | 1197 | C    |
| 2   | S60   | 1198 | U    |
| 2   | S60   | 1199 | C    |
| 2   | S60   | 1200 | A    |
| 2   | S60   | 1202 | U    |
| 2   | S60   | 1203 | A    |
| 2   | S60   | 1204 | A    |
| 2   | S60   | 1205 | G    |
| 2   | S60   | 1206 | A    |
| 2   | S60   | 1207 | A    |
| 2   | S60   | 1208 | G    |
| 2   | S60   | 1209 | C    |
| 2   | S60   | 1210 | G    |
| 2   | S60   | 1211 | A    |
| 2   | S60   | 1214 | A    |
| 2   | S60   | 1215 | A    |
| 2   | S60   | 1216 | U    |
| 2   | S60   | 1217 | G    |
| 2   | S60   | 1221 | C    |
| 2   | S60   | 1223 | C    |
| 2   | S60   | 1225 | G    |
| 2   | S60   | 1230 | U    |
| 2   | S60   | 1232 | G    |
| 2   | S60   | 1233 | U    |
| 2   | S60   | 1237 | C    |
| 2   | S60   | 1239 | C    |
| 2   | S60   | 1240 | C    |
| 2   | S60   | 1248 | G    |
| 2   | S60   | 1250 | U    |
| 2   | S60   | 1251 | A    |
| 2   | S60   | 1260 | G    |
| 2   | S60   | 1262 | A    |
| 2   | S60   | 1263 | A    |
| 2   | S60   | 1266 | A    |
| 2   | S60   | 1267 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S60   | 1274 | A    |
| 2   | S60   | 1283 | A    |
| 2   | S60   | 1284 | G    |
| 2   | S60   | 1287 | A    |
| 2   | S60   | 1291 | A    |
| 2   | S60   | 1292 | G    |
| 2   | S60   | 1294 | G    |
| 2   | S60   | 1295 | C    |
| 2   | S60   | 1296 | A    |
| 2   | S60   | 1297 | G    |
| 2   | S60   | 1298 | G    |
| 2   | S60   | 1300 | U    |
| 2   | S60   | 1301 | U    |
| 2   | S60   | 1302 | C    |
| 2   | S60   | 1303 | U    |
| 2   | S60   | 1308 | C    |
| 2   | S60   | 1310 | G    |
| 2   | S60   | 1312 | U    |
| 2   | S60   | 1313 | A    |
| 2   | S60   | 1314 | C    |
| 2   | S60   | 1315 | A    |
| 2   | S60   | 1316 | A    |
| 2   | S60   | 1317 | G    |
| 2   | S60   | 1319 | C    |
| 2   | S60   | 1320 | G    |
| 2   | S60   | 1322 | A    |
| 2   | S60   | 1325 | A    |
| 2   | S60   | 1326 | A    |
| 2   | S60   | 1327 | G    |
| 2   | S60   | 1328 | G    |
| 2   | S60   | 1329 | C    |
| 2   | S60   | 1340 | G    |
| 2   | S60   | 1342 | A    |
| 2   | S60   | 1343 | C    |
| 2   | S60   | 1346 | G    |
| 2   | S60   | 1352 | G    |
| 2   | S60   | 1354 | A    |
| 2   | S60   | 1355 | U    |
| 2   | S60   | 1356 | C    |
| 2   | S60   | 1357 | A    |
| 7   | L70   | 2    | G    |
| 7   | L70   | 3    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | L70   | 4   | U    |
| 7   | L70   | 5   | A    |
| 7   | L70   | 7   | G    |
| 7   | L70   | 14  | U    |
| 7   | L70   | 17  | A    |
| 7   | L70   | 22  | A    |
| 7   | L70   | 26  | C    |
| 7   | L70   | 27  | A    |
| 7   | L70   | 28  | C    |
| 7   | L70   | 29  | C    |
| 7   | L70   | 33  | U    |
| 7   | L70   | 34  | C    |
| 7   | L70   | 41  | G    |
| 7   | L70   | 42  | A    |
| 7   | L70   | 45  | U    |
| 7   | L70   | 49  | A    |
| 7   | L70   | 50  | A    |
| 7   | L70   | 54  | A    |
| 7   | L70   | 55  | A    |
| 7   | L70   | 63  | A    |
| 7   | L70   | 64  | G    |
| 7   | L70   | 67  | C    |
| 7   | L70   | 76  | U    |
| 7   | L70   | 91  | C    |
| 7   | L70   | 100 | A    |
| 7   | L70   | 101 | A    |
| 7   | L70   | 110 | G    |

All (224) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 1   | A    |
| 1   | K50   | 14  | G    |
| 1   | K50   | 21  | U    |
| 1   | K50   | 75  | C    |
| 1   | K50   | 150 | G    |
| 1   | K50   | 156 | G    |
| 1   | K50   | 166 | A    |
| 1   | K50   | 201 | A    |
| 1   | K50   | 225 | G    |
| 1   | K50   | 242 | A    |
| 1   | K50   | 308 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 311  | C    |
| 1   | K50   | 330  | G    |
| 1   | K50   | 494  | A    |
| 1   | K50   | 536  | A    |
| 1   | K50   | 548  | G    |
| 1   | K50   | 562  | U    |
| 1   | K50   | 667  | G    |
| 1   | K50   | 723  | G    |
| 1   | K50   | 904  | A    |
| 1   | K50   | 921  | A    |
| 1   | K50   | 924  | G    |
| 1   | K50   | 934  | U    |
| 1   | K50   | 952  | A    |
| 1   | K50   | 956  | A    |
| 1   | K50   | 970  | U    |
| 1   | K50   | 971  | A    |
| 1   | K50   | 972  | C    |
| 1   | K50   | 1134 | A    |
| 1   | K50   | 1148 | A    |
| 1   | K50   | 1277 | G    |
| 1   | K50   | 1394 | U    |
| 1   | K50   | 1395 | U    |
| 1   | K50   | 1415 | G    |
| 1   | K50   | 1491 | U    |
| 1   | K50   | 1686 | G    |
| 1   | K50   | 1733 | A    |
| 1   | K50   | 1835 | G    |
| 1   | K50   | 1875 | G    |
| 1   | K50   | 1883 | A    |
| 1   | K50   | 1898 | G    |
| 1   | K50   | 1904 | A    |
| 1   | K50   | 1928 | C    |
| 1   | K50   | 1929 | U    |
| 1   | K50   | 1946 | G    |
| 1   | K50   | 1950 | C    |
| 1   | K50   | 2109 | G    |
| 1   | K50   | 2205 | G    |
| 1   | K50   | 2267 | C    |
| 1   | K50   | 2268 | A    |
| 1   | K50   | 2269 | G    |
| 1   | K50   | 2452 | A    |
| 1   | K50   | 2470 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2481 | U    |
| 1   | K50   | 2486 | U    |
| 1   | K50   | 2597 | G    |
| 2   | R60   | 1    | A    |
| 2   | R60   | 17   | C    |
| 2   | R60   | 56   | U    |
| 2   | R60   | 67   | C    |
| 2   | R60   | 74   | U    |
| 2   | R60   | 78   | G    |
| 2   | R60   | 83   | G    |
| 2   | R60   | 141  | G    |
| 2   | R60   | 149  | A    |
| 2   | R60   | 180  | G    |
| 2   | R60   | 193  | G    |
| 2   | R60   | 262  | U    |
| 2   | R60   | 319  | A    |
| 2   | R60   | 355  | C    |
| 2   | R60   | 362  | G    |
| 2   | R60   | 363  | C    |
| 2   | R60   | 383  | A    |
| 2   | R60   | 391  | U    |
| 2   | R60   | 408  | A    |
| 2   | R60   | 417  | A    |
| 2   | R60   | 420  | U    |
| 2   | R60   | 421  | C    |
| 2   | R60   | 425  | G    |
| 2   | R60   | 447  | A    |
| 2   | R60   | 448  | U    |
| 2   | R60   | 473  | G    |
| 2   | R60   | 565  | U    |
| 2   | R60   | 738  | A    |
| 2   | R60   | 780  | G    |
| 2   | R60   | 825  | U    |
| 2   | R60   | 872  | U    |
| 2   | R60   | 873  | C    |
| 2   | R60   | 874  | A    |
| 2   | R60   | 877  | G    |
| 2   | R60   | 911  | G    |
| 2   | R60   | 913  | G    |
| 2   | R60   | 915  | A    |
| 2   | R60   | 989  | G    |
| 2   | R60   | 1002 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | R60   | 1018 | U    |
| 2   | R60   | 1021 | A    |
| 2   | R60   | 1023 | A    |
| 2   | R60   | 1033 | A    |
| 2   | R60   | 1041 | A    |
| 2   | R60   | 1044 | G    |
| 2   | R60   | 1132 | A    |
| 2   | R60   | 1135 | U    |
| 2   | R60   | 1191 | C    |
| 2   | R60   | 1196 | U    |
| 2   | R60   | 1203 | A    |
| 2   | R60   | 1210 | G    |
| 2   | R60   | 1311 | A    |
| 2   | R60   | 1313 | A    |
| 2   | R60   | 1314 | C    |
| 7   | K70   | 48   | G    |
| 7   | K70   | 49   | A    |
| 1   | L50   | 1    | A    |
| 1   | L50   | 14   | G    |
| 1   | L50   | 21   | U    |
| 1   | L50   | 75   | C    |
| 1   | L50   | 150  | G    |
| 1   | L50   | 156  | G    |
| 1   | L50   | 166  | A    |
| 1   | L50   | 201  | A    |
| 1   | L50   | 225  | G    |
| 1   | L50   | 242  | A    |
| 1   | L50   | 308  | A    |
| 1   | L50   | 311  | C    |
| 1   | L50   | 330  | G    |
| 1   | L50   | 494  | A    |
| 1   | L50   | 536  | A    |
| 1   | L50   | 548  | G    |
| 1   | L50   | 562  | U    |
| 1   | L50   | 667  | G    |
| 1   | L50   | 723  | G    |
| 1   | L50   | 904  | A    |
| 1   | L50   | 921  | A    |
| 1   | L50   | 924  | G    |
| 1   | L50   | 934  | U    |
| 1   | L50   | 952  | A    |
| 1   | L50   | 956  | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 970  | U    |
| 1   | L50   | 971  | A    |
| 1   | L50   | 972  | C    |
| 1   | L50   | 1134 | A    |
| 1   | L50   | 1148 | A    |
| 1   | L50   | 1277 | G    |
| 1   | L50   | 1394 | U    |
| 1   | L50   | 1395 | U    |
| 1   | L50   | 1415 | G    |
| 1   | L50   | 1491 | U    |
| 1   | L50   | 1686 | G    |
| 1   | L50   | 1733 | A    |
| 1   | L50   | 1835 | G    |
| 1   | L50   | 1875 | G    |
| 1   | L50   | 1883 | A    |
| 1   | L50   | 1898 | G    |
| 1   | L50   | 1904 | A    |
| 1   | L50   | 1928 | C    |
| 1   | L50   | 1929 | U    |
| 1   | L50   | 1946 | G    |
| 1   | L50   | 1950 | C    |
| 1   | L50   | 2109 | G    |
| 1   | L50   | 2205 | G    |
| 1   | L50   | 2267 | C    |
| 1   | L50   | 2268 | A    |
| 1   | L50   | 2269 | G    |
| 1   | L50   | 2452 | A    |
| 1   | L50   | 2470 | C    |
| 1   | L50   | 2481 | U    |
| 1   | L50   | 2486 | U    |
| 1   | L50   | 2597 | G    |
| 2   | S60   | 1    | A    |
| 2   | S60   | 17   | C    |
| 2   | S60   | 56   | U    |
| 2   | S60   | 67   | C    |
| 2   | S60   | 74   | U    |
| 2   | S60   | 78   | G    |
| 2   | S60   | 83   | G    |
| 2   | S60   | 141  | G    |
| 2   | S60   | 149  | A    |
| 2   | S60   | 180  | G    |
| 2   | S60   | 193  | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S60   | 262  | U    |
| 2   | S60   | 319  | A    |
| 2   | S60   | 355  | C    |
| 2   | S60   | 362  | G    |
| 2   | S60   | 363  | C    |
| 2   | S60   | 383  | A    |
| 2   | S60   | 391  | U    |
| 2   | S60   | 408  | A    |
| 2   | S60   | 417  | A    |
| 2   | S60   | 420  | U    |
| 2   | S60   | 421  | C    |
| 2   | S60   | 425  | G    |
| 2   | S60   | 447  | A    |
| 2   | S60   | 448  | U    |
| 2   | S60   | 473  | G    |
| 2   | S60   | 565  | U    |
| 2   | S60   | 738  | A    |
| 2   | S60   | 780  | G    |
| 2   | S60   | 825  | U    |
| 2   | S60   | 872  | U    |
| 2   | S60   | 873  | C    |
| 2   | S60   | 874  | A    |
| 2   | S60   | 877  | G    |
| 2   | S60   | 911  | G    |
| 2   | S60   | 913  | G    |
| 2   | S60   | 915  | A    |
| 2   | S60   | 989  | G    |
| 2   | S60   | 1002 | U    |
| 2   | S60   | 1018 | U    |
| 2   | S60   | 1021 | A    |
| 2   | S60   | 1023 | A    |
| 2   | S60   | 1033 | A    |
| 2   | S60   | 1041 | A    |
| 2   | S60   | 1044 | G    |
| 2   | S60   | 1132 | A    |
| 2   | S60   | 1135 | U    |
| 2   | S60   | 1191 | C    |
| 2   | S60   | 1196 | U    |
| 2   | S60   | 1203 | A    |
| 2   | S60   | 1210 | G    |
| 2   | S60   | 1311 | A    |
| 2   | S60   | 1313 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S60   | 1314 | C    |
| 7   | L70   | 48   | G    |
| 7   | L70   | 49   | A    |

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

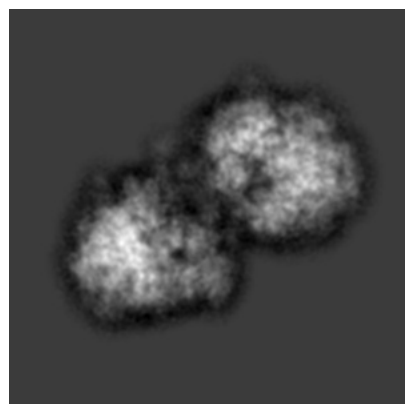
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55401. These allow visual inspection of the internal detail of the map and identification of artifacts.

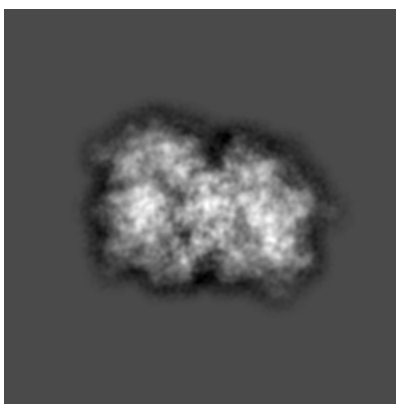
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

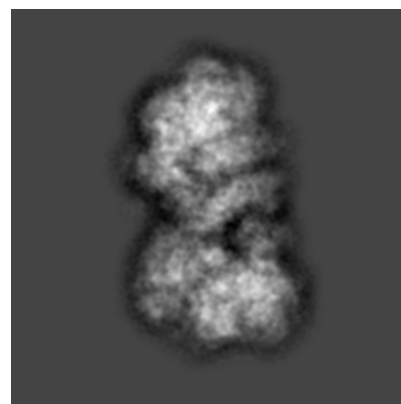
#### 6.1.1 Primary map



X

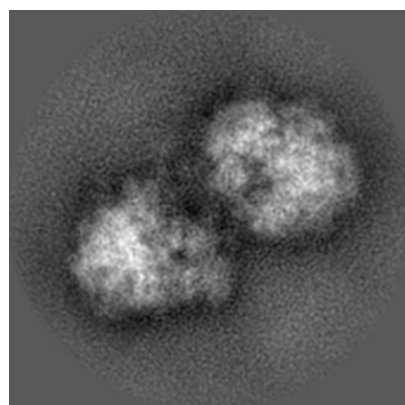


Y

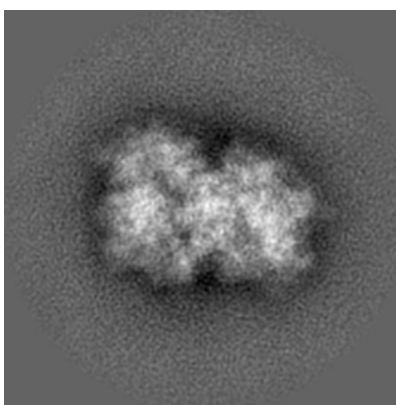


Z

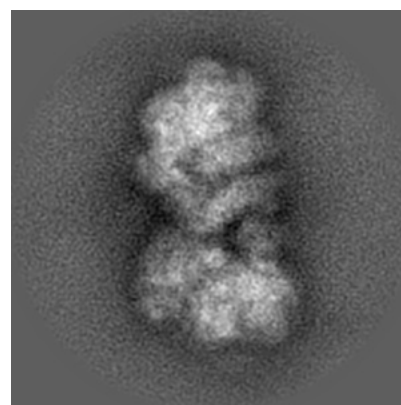
#### 6.1.2 Raw map



X



Y

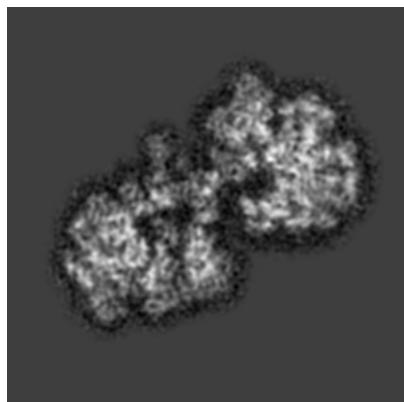


Z

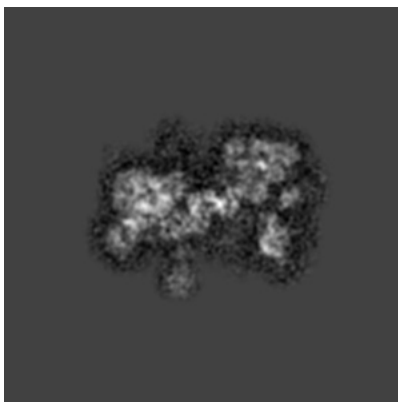
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

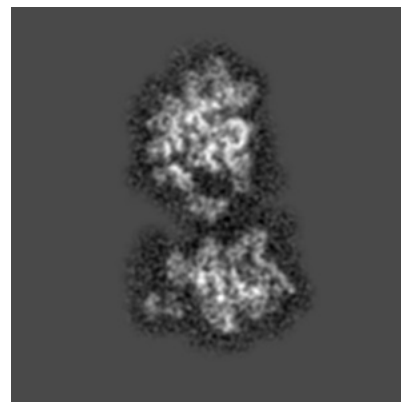
### 6.2.1 Primary map



X Index: 84

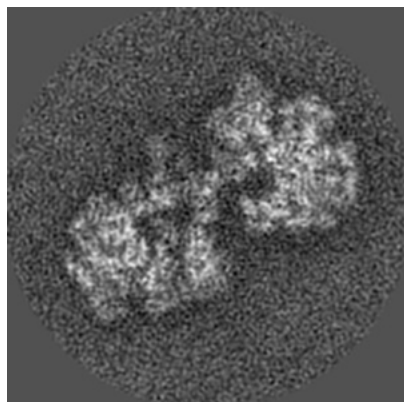


Y Index: 84

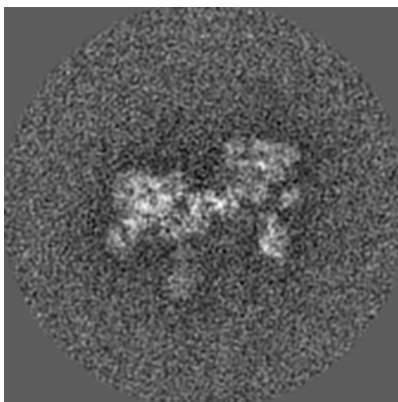


Z Index: 84

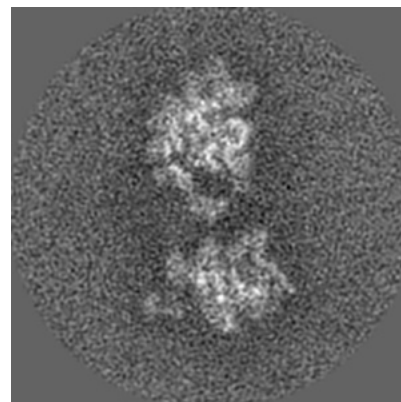
### 6.2.2 Raw map



X Index: 84



Y Index: 84

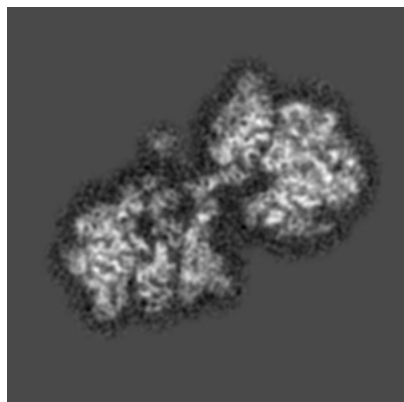


Z Index: 84

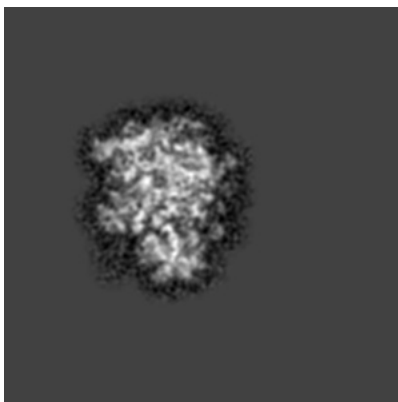
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

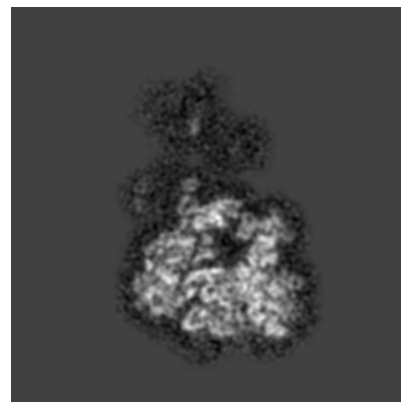
### 6.3.1 Primary map



X Index: 81

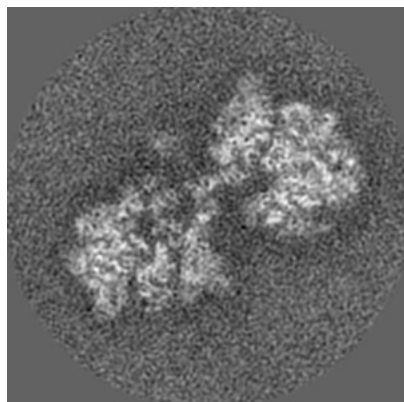


Y Index: 47

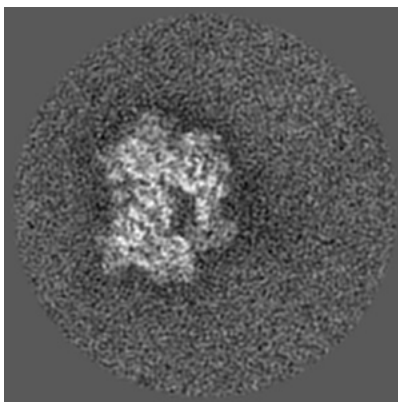


Z Index: 68

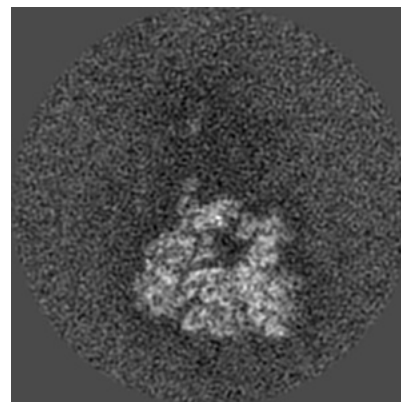
### 6.3.2 Raw map



X Index: 81



Y Index: 55

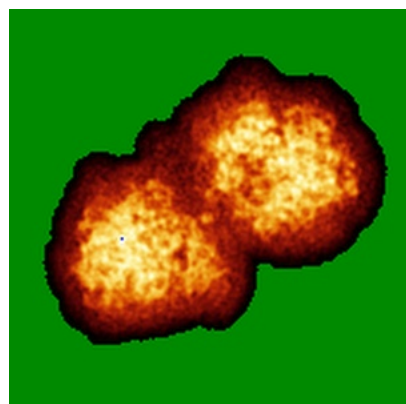


Z Index: 68

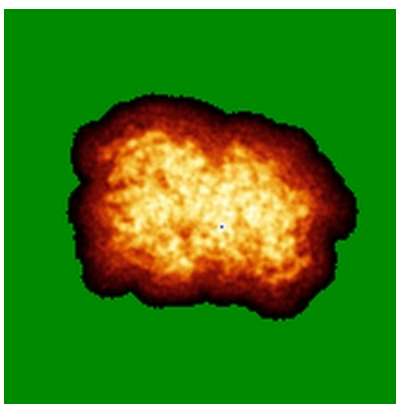
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

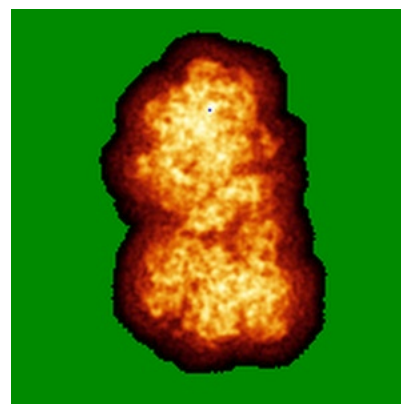
### 6.4.1 Primary map



X

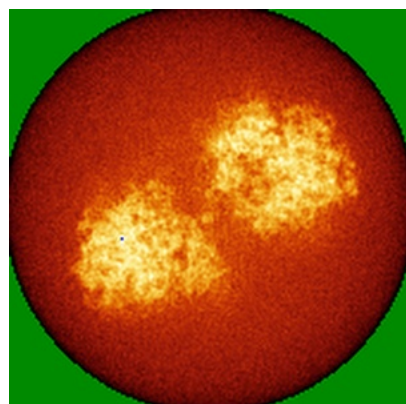


Y

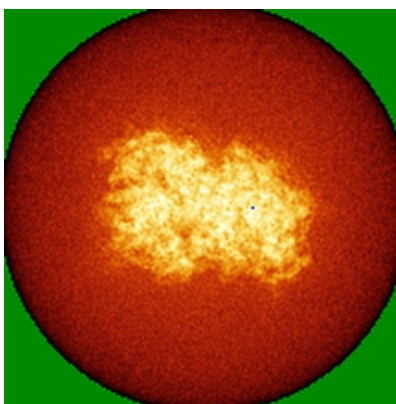


Z

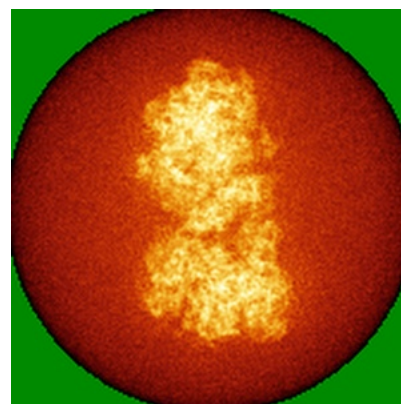
### 6.4.2 Raw map



X



Y

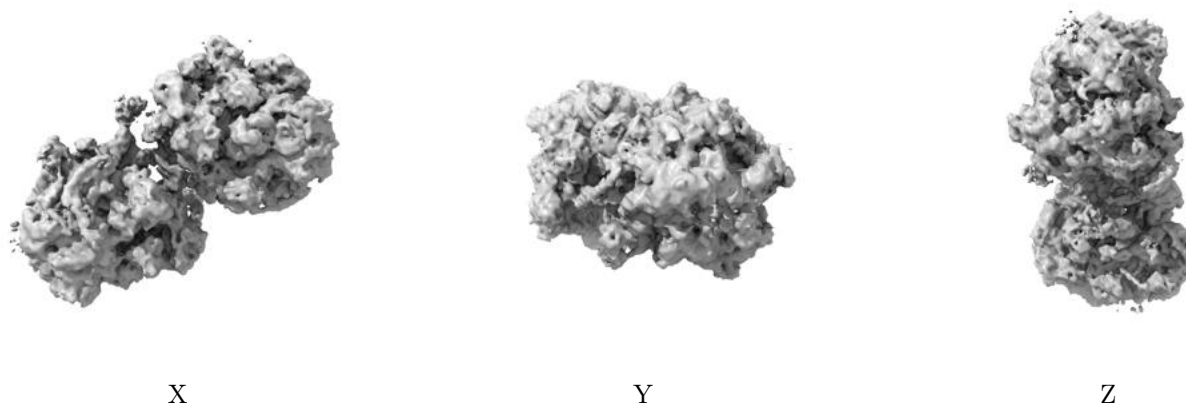


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

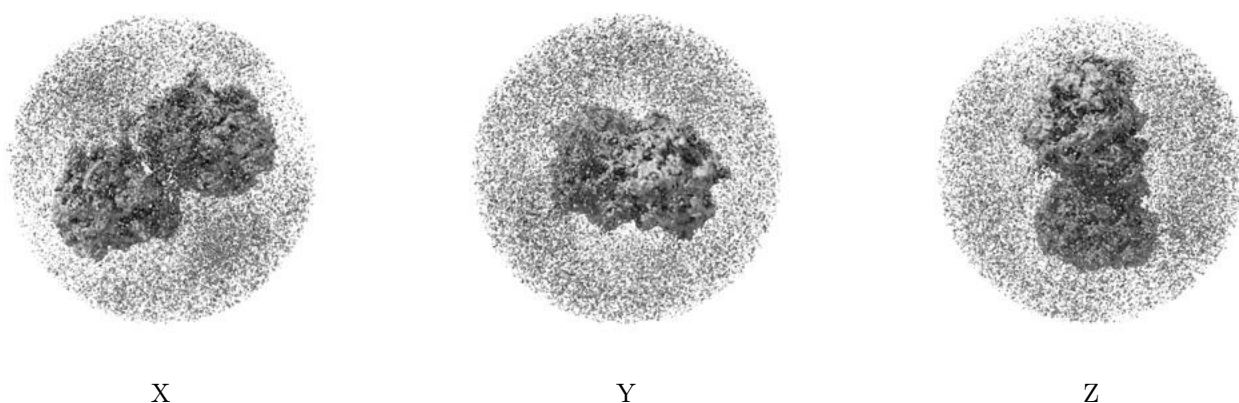
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

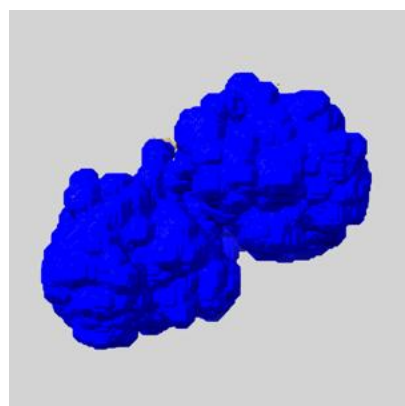
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

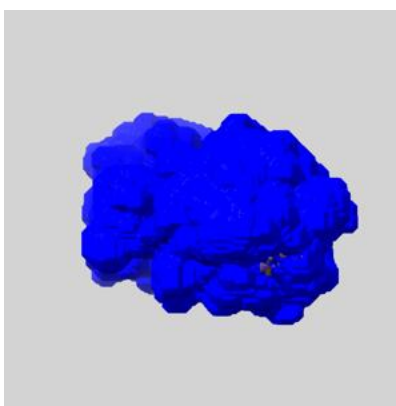
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

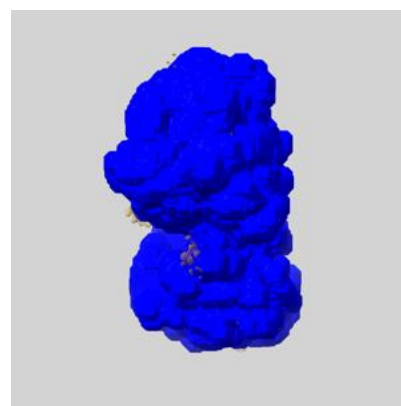
### 6.6.1 emd\_55401\_msk\_1.map [i](#)



X



Y

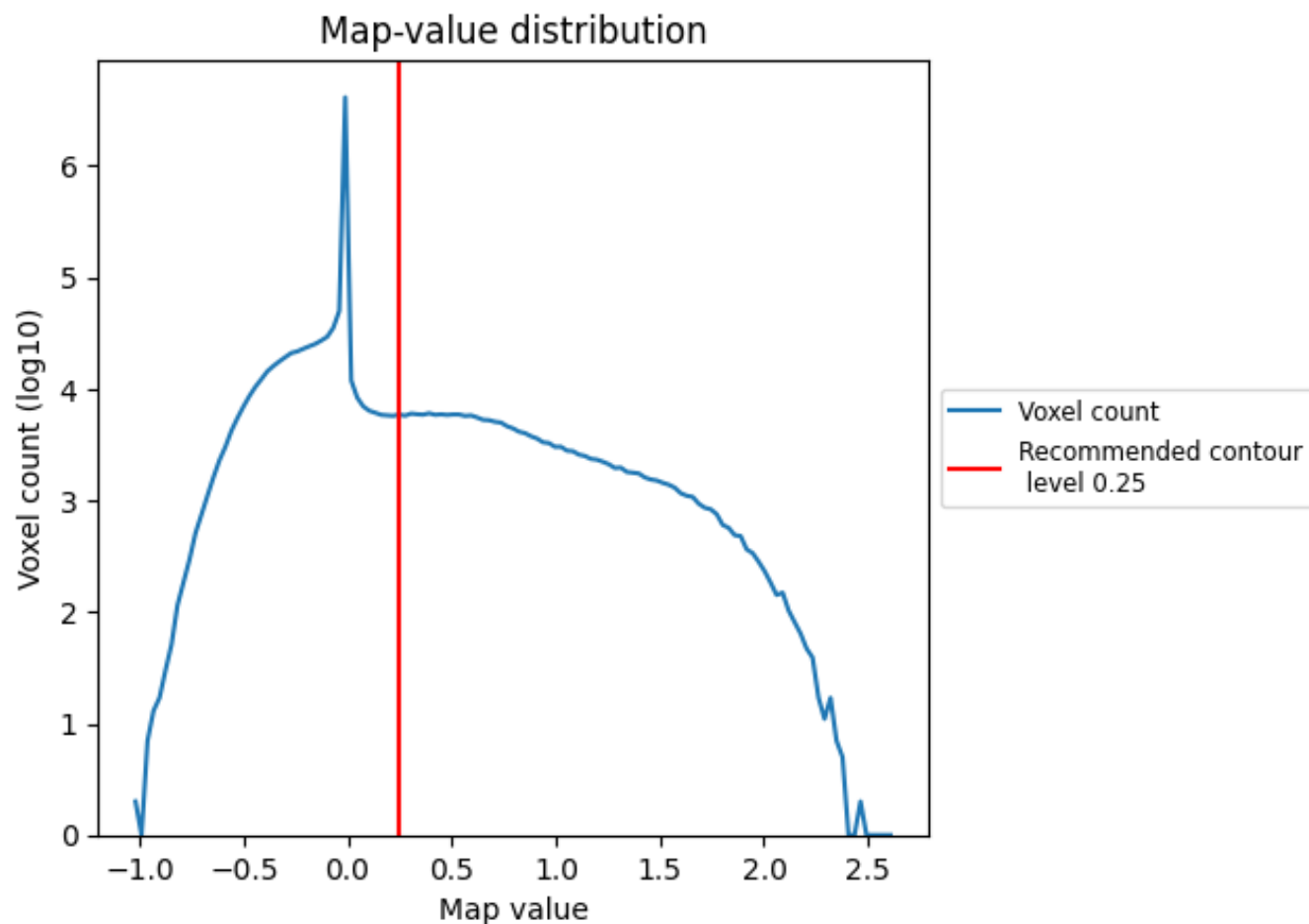


Z

## 7 Map analysis [i](#)

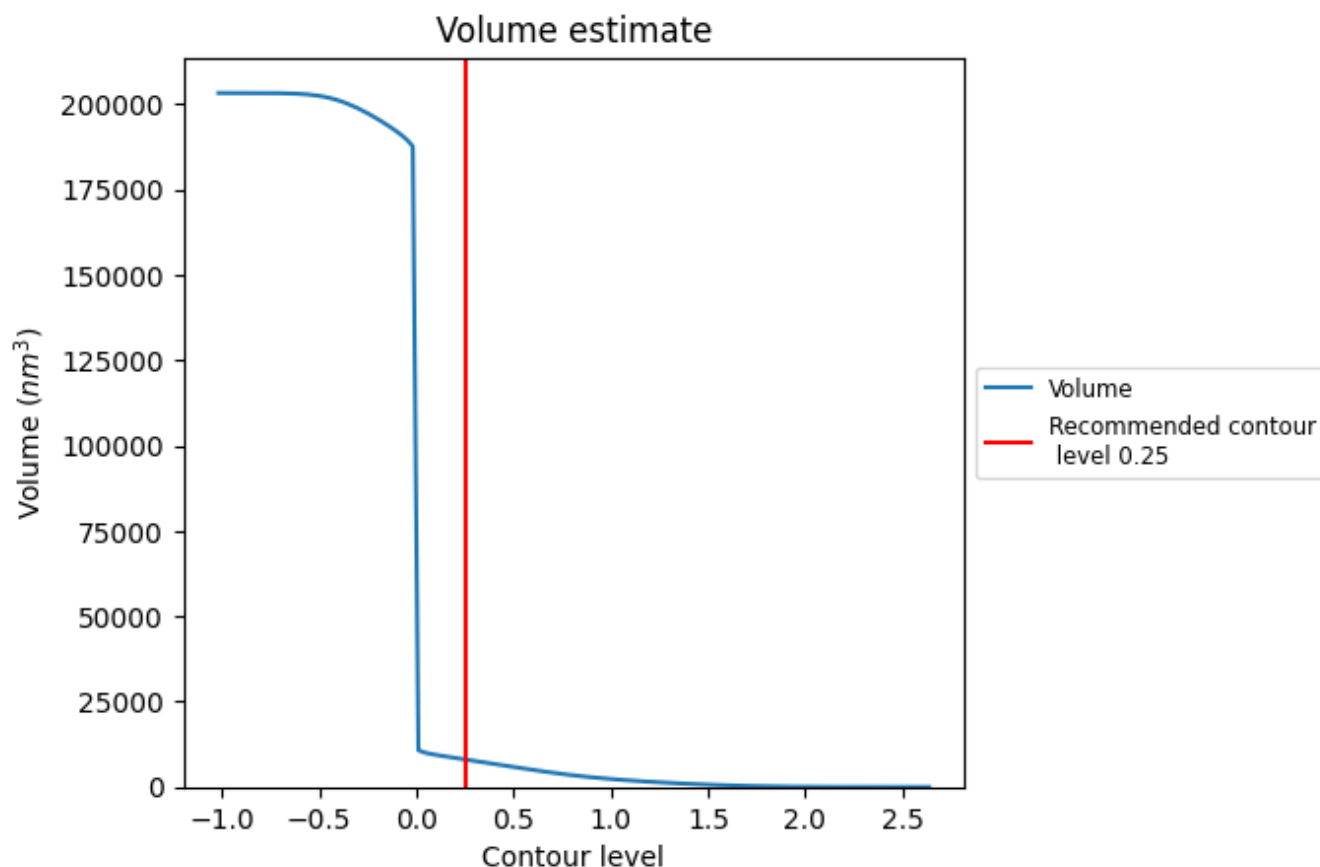
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

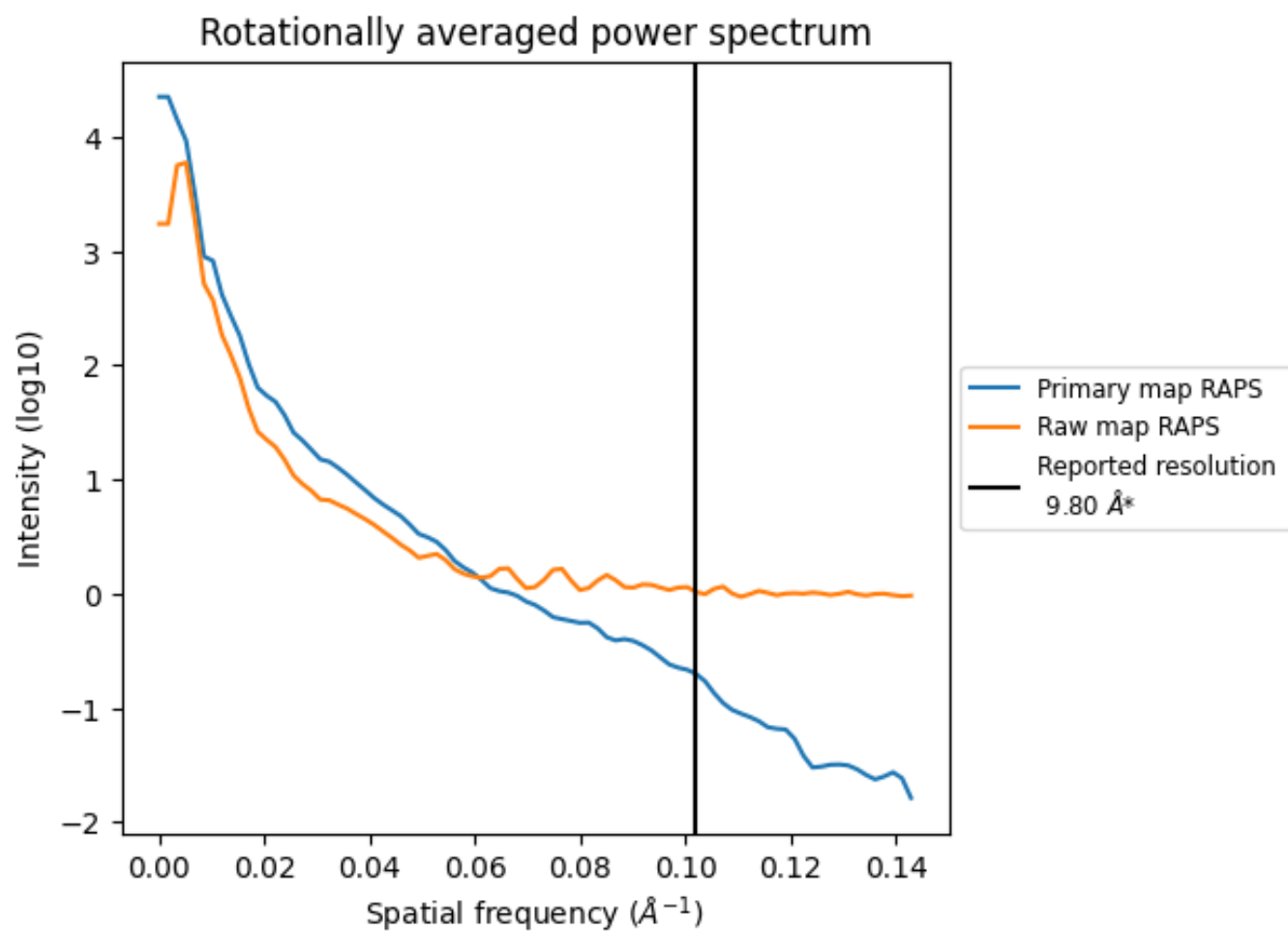
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8050  $\text{nm}^3$ ; this corresponds to an approximate mass of 7272 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

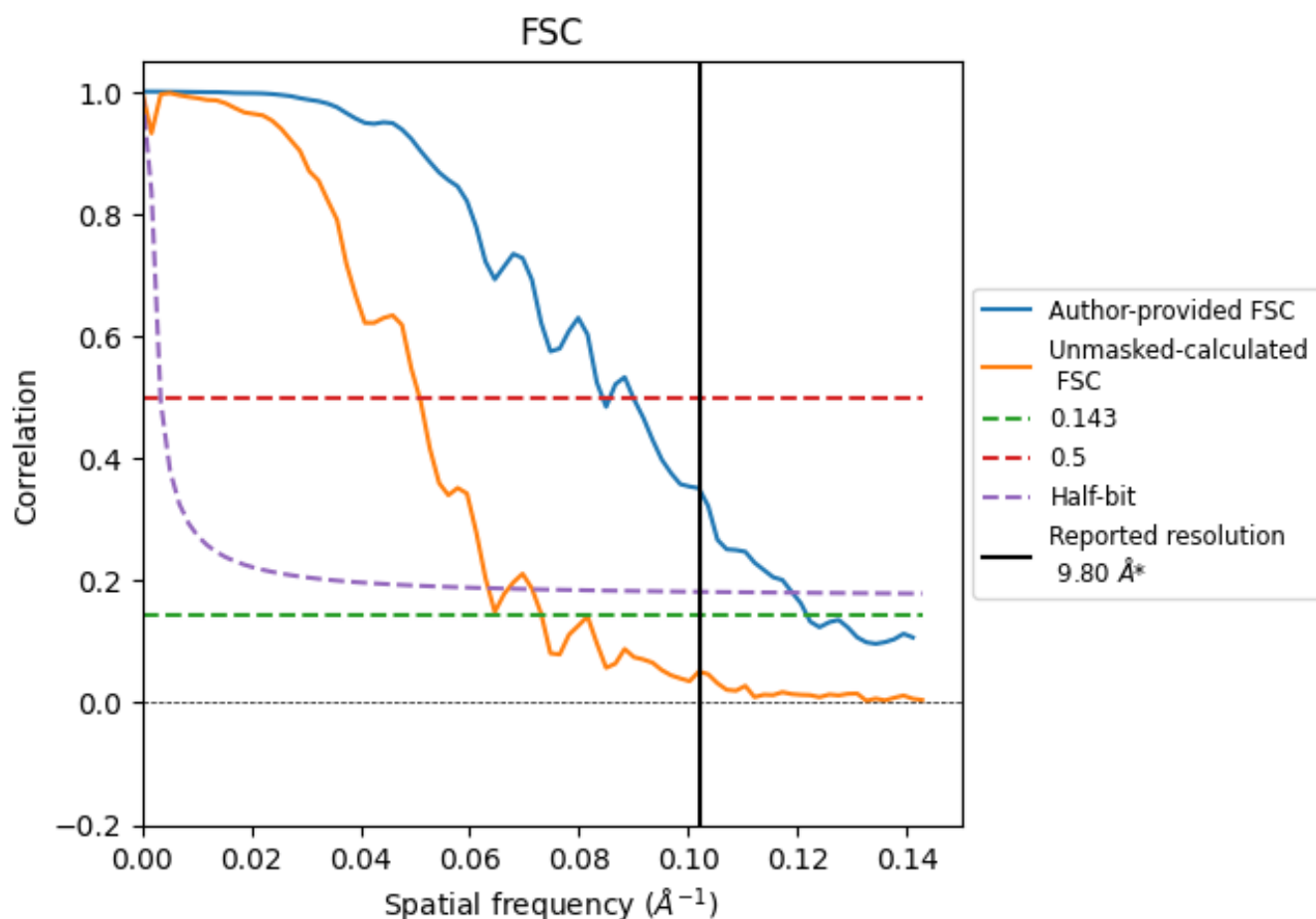


\*Reported resolution corresponds to spatial frequency of 0.102 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.102 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 9.80                               | -     | -        |
| Author-provided FSC curve | 8.20                               | 11.85 | 8.39     |
| Unmasked-calculated*      | 13.66                              | 19.69 | 15.77    |

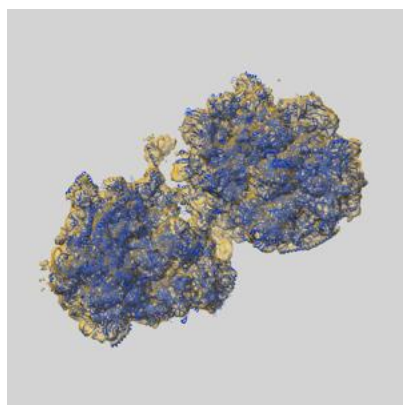
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.20 differs from the reported value 9.8 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.66 differs from the reported value 9.8 by more than 10 %

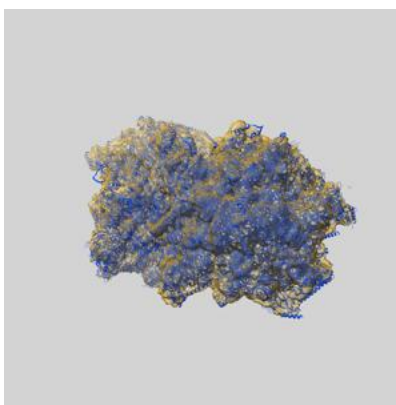
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55401 and PDB model 9T0I. Per-residue inclusion information can be found in section 3 on page 26.

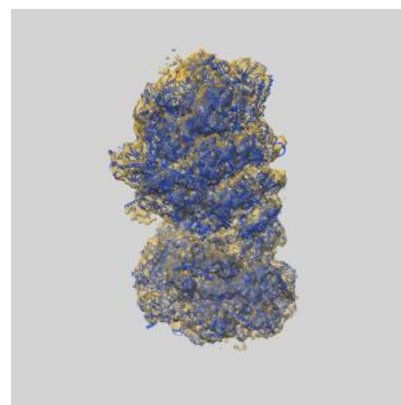
### 9.1 Map-model overlay [i](#)



X



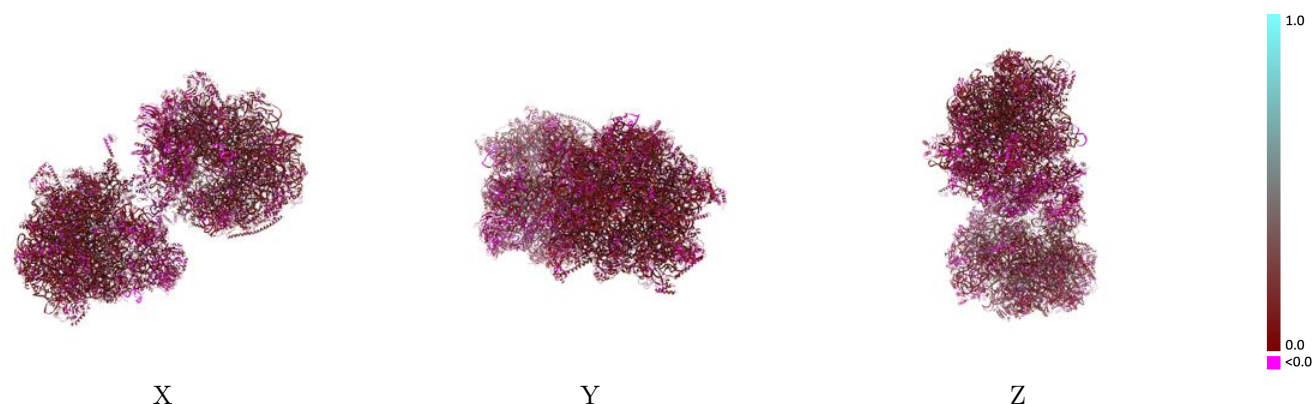
Y



Z

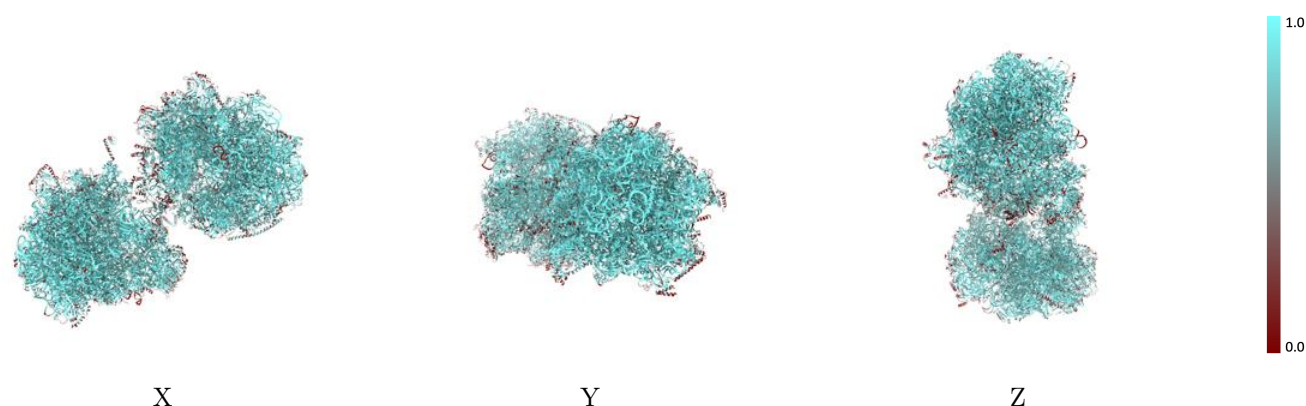
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



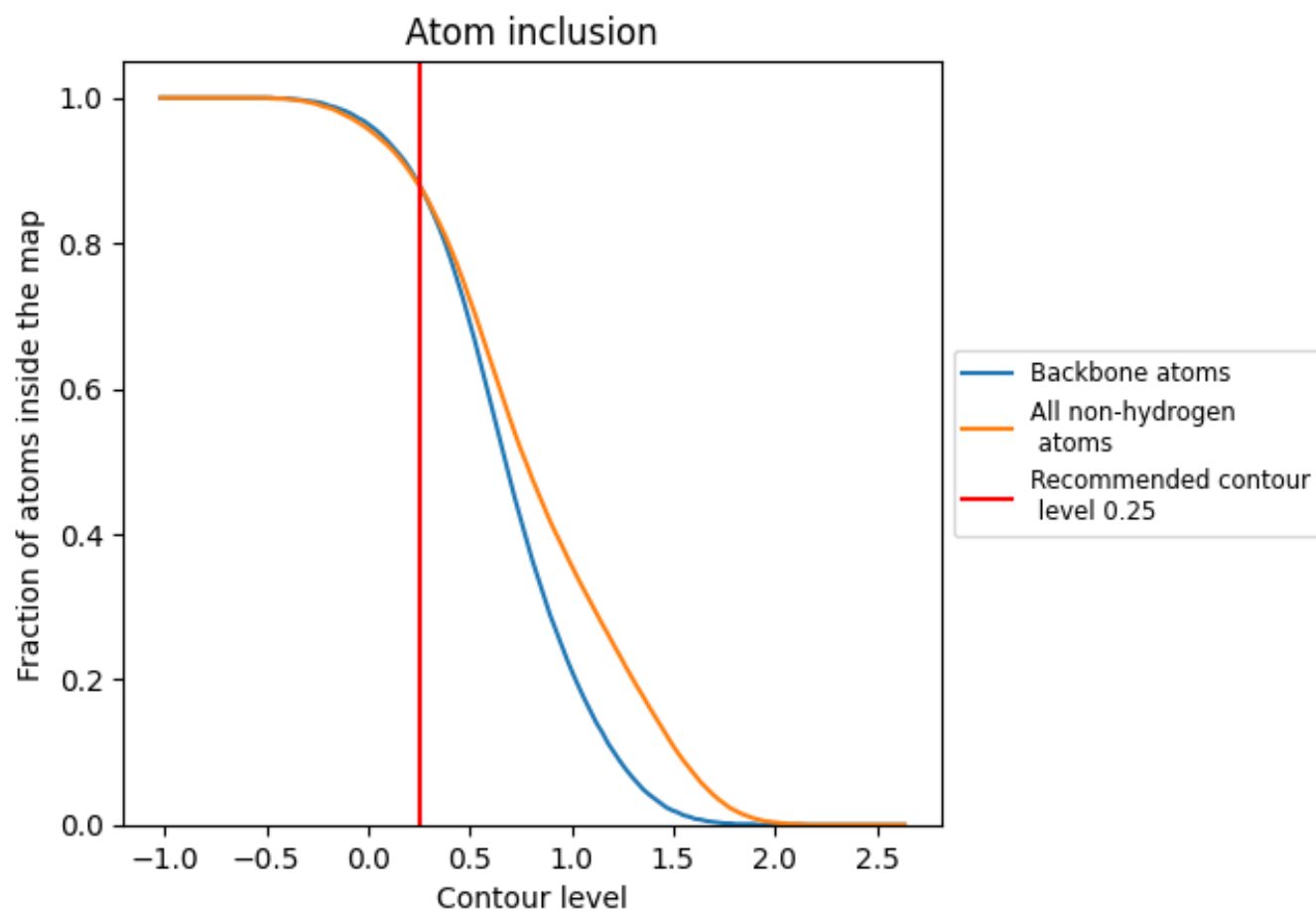
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8800   |  0.1010   |
| A     |  0.8330   |  0.1060   |
| B     |  0.7730   |  0.1040   |
| D     |  0.7540   |  0.1350   |
| E     |  0.7450   |  0.1180   |
| K     |  0.7740   |  0.0850   |
| K50   |  0.9840   |  0.1380   |
| K70   |  0.9720   |  0.1290   |
| KAA   |  0.9010   |  0.0550   |
| KB0   |  0.8260   |  0.0710   |
| KC0   |  0.8140   |  0.0570   |
| KCC   |  0.7890   |  0.1120   |
| KD0   |  0.7750   |  0.0540   |
| KDD   |  0.8740   |  0.0920   |
| KE0   |  0.5890  |  0.0720  |
| KEE   |  0.8380 |  0.0570 |
| KF0   |  0.7980 |  0.1010 |
| KFF   |  0.8880 |  0.0860 |
| KG0   |  0.7330 |  0.0890 |
| KGG   |  0.9260 |  0.0580 |
| KH0   |  0.8050 |  0.0960 |
| KHH   |  0.8330 |  0.1240 |
| KI0   |  0.8380 |  0.0910 |
| KII   |  0.7490 |  0.0860 |
| KJ0   |  0.8610 |  0.0660 |
| KJJ   |  0.9750 |  0.0720 |
| KL0   |  0.8260 |  0.0640 |
| KLL   |  0.9850 |  0.0700 |
| KM0   |  0.7140 |  0.1270 |
| KMM   |  0.7730 |  0.0710 |
| KN0   |  0.9820 |  0.0500 |
| KO0   |  0.7890 |  0.1110 |
| KOO   |  0.8380 |  0.0630 |
| KP0   |  0.8990 |  0.1000 |
| KPP   |  0.8970 |  0.0950 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| KQ0   |  0.8170   |  0.0910   |
| KR0   |  0.8230   |  0.1050   |
| KS0   |  0.7590   |  0.0980   |
| KT0   |  0.7690   |  0.0690   |
| KU0   |  0.7770   |  0.1030   |
| KV0   |  0.8520   |  0.0830   |
| KW0   |  0.6530   |  0.0660   |
| KX0   |  0.8560   |  0.0750   |
| KY0   |  0.8570   |  0.0750   |
| KZ0   |  0.6950   |  0.0830   |
| L     |  0.8250   |  0.0790   |
| L50   |  0.9870   |  0.1400   |
| L70   |  0.9820   |  0.1150   |
| LA0   |  0.8730   |  0.0730   |
| LA02  |  0.9070   |  0.0850   |
| LAA   |  0.8940   |  0.0550   |
| LB0   |  0.8800   |  0.0730   |
| LC0   |  0.8270  |  0.0660  |
| LCC   |  0.8330 |  0.1230 |
| LD0   |  0.7350 |  0.0540 |
| LDD   |  0.8720 |  0.0900 |
| LE0   |  0.6550 |  0.0800 |
| LEE   |  0.8690 |  0.0660 |
| LF0   |  0.8210 |  0.1020 |
| LFF   |  0.8820 |  0.0960 |
| LG0   |  0.7740 |  0.1060 |
| LGG   |  0.9420 |  0.0540 |
| LH0   |  0.8280 |  0.1080 |
| LHH   |  0.8640 |  0.1130 |
| LI0   |  0.8800 |  0.0930 |
| LII   |  0.7730 |  0.1130 |
| LJ0   |  0.8510 |  0.0550 |
| LJJ   |  0.9620 |  0.0890 |
| LL0   |  0.8700 |  0.0800 |
| LLL   |  1.0000 |  0.0900 |
| LM0   |  0.7460 |  0.1190 |
| LMM   |  0.8390 |  0.0770 |
| LN0   |  0.9970 |  0.0520 |
| LO0   |  0.8380 |  0.1200 |
| LOO   |  0.8780 |  0.0760 |
| LP0   |  0.9190 |  0.0920 |
| LPP   |  0.9220 |  0.1110 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| LQ0   |  0.8290   |  0.0890    |
| LR0   |  0.8600   |  0.1040    |
| LS0   |  0.8010   |  0.0940    |
| LT0   |  0.7890   |  0.0700    |
| LU0   |  0.7840   |  0.0920    |
| LV0   |  0.9200   |  0.0720    |
| LW0   |  0.6720   |  0.0810    |
| LX0   |  0.8960   |  0.0730    |
| LY0   |  0.8730   |  0.0860    |
| LZ0   |  0.7390   |  0.0910    |
| M     |  0.7390   |  0.0950    |
| MD1   |  0.8650   |  0.1070    |
| N     |  0.7360   |  0.1110    |
| ND1   |  0.7870   |  0.1090    |
| R60   |  0.9740   |  0.1080    |
| RA0   |  0.7270   |  0.0400    |
| RAA   |  0.8320   |  0.0800    |
| RB0   |  0.7850   |  0.1130    |
| RBB   |  0.7100  |  0.0660   |
| RC0   |  0.7930 |  0.0710  |
| RCC   |  0.7090 |  0.0740  |
| RD0   |  0.5250 |  0.0250  |
| RDD   |  0.7820 |  0.0720  |
| RE0   |  0.7000 |  0.0430  |
| REE   |  0.7320 |  0.0540  |
| RF0   |  0.8580 |  0.0460  |
| RFF   |  0.5070 |  -0.0030 |
| RG0   |  0.6240 |  0.0500  |
| RGG   |  0.6400 |  0.0260  |
| RH0   |  0.5990 |  0.0660  |
| RI0   |  0.8430 |  0.0430  |
| RJ0   |  0.7690 |  0.0480  |
| RK0   |  0.6180 |  0.0200  |
| RL0   |  0.6860 |  0.0600  |
| RM0   |  0.3540 |  0.0260  |
| RN0   |  0.8400 |  0.0650  |
| RO0   |  0.8810 |  0.0780  |
| RP0   |  0.7210 |  0.0530  |
| RQ0   |  0.8040 |  0.0520  |
| RR0   |  0.6730 |  0.0390  |
| RS0   |  0.8390 |  0.0560  |
| RT0   |  0.7340 |  0.0700  |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| RU0   |  0.6260   |  0.0510   |
| RV0   |  0.7890   |  0.0840   |
| RW0   |  0.8510   |  0.0600   |
| RX0   |  0.9110   |  0.0810   |
| RY0   |  0.6390   |  0.0380   |
| RZ0   |  0.8070   |  0.0730   |
| S60   |  0.9770   |  0.1120   |
| SA0   |  0.7680   |  0.0480   |
| SAA   |  0.8710   |  0.0790   |
| SB0   |  0.8360   |  0.1250   |
| SBB   |  0.6870   |  0.0760   |
| SC0   |  0.8110   |  0.0790   |
| SCC   |  0.7370   |  0.0930   |
| SD0   |  0.5490   |  0.0300   |
| SDD   |  0.8060   |  0.0890   |
| SE0   |  0.6990   |  0.0470   |
| SEE   |  0.7610   |  0.0630   |
| SF0   |  0.8670   |  0.0510   |
| SFF   |  0.5420  |  0.0240  |
| SG0   |  0.6510 |  0.0580 |
| SGG   |  0.6330 |  0.0410 |
| SH0   |  0.6220 |  0.0700 |
| SI0   |  0.8800 |  0.0540 |
| SJ0   |  0.7730 |  0.0570 |
| SK0   |  0.6810 |  0.0550 |
| SL0   |  0.7230 |  0.0820 |
| SM0   |  0.3150 |  0.0060 |
| SN0   |  0.8680 |  0.0840 |
| SO0   |  0.9100 |  0.0560 |
| SP0   |  0.6930 |  0.0460 |
| SQ0   |  0.8120 |  0.0510 |
| SR0   |  0.6700 |  0.0630 |
| SS0   |  0.8360 |  0.0480 |
| ST0   |  0.7070 |  0.0380 |
| SU0   |  0.6430 |  0.0310 |
| SV0   |  0.8230 |  0.1130 |
| SW0   |  0.8980 |  0.0590 |
| SX0   |  0.9410 |  0.0640 |
| SY0   |  0.6360 |  0.0480 |
| SZ0   |  0.7820 |  0.0580 |